Solution of the Skyrme-Hartree-Fock equations in the Cartesian deformed harmonic oscillator basis. (II) The program HFODD.

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Abstract

We describe the code HFODD which solves the nuclear Skyrme-Hartree-Fock problem by using the deformed Cartesian harmonic oscillator basis. The user has a possibility of choosing among various symmetries of the nuclear HF problem for rotating or non-rotating nuclei; they vary from the non-axial parity-invariant nuclear shapes, through those also breaking the intrinsic parity, towards the least-restrictive case corresponding to only one symmetry plane. The code provides a solution for a complete superdeformed rotational band in an $A{\sim}150$ nucleus within one CPU hour of the CRAY C-90 supercomputer or within two-three CPU hours of a fast workstation.

PROGRAM SUMMARY

Title of the program: HFODD (v1.60n)

Catalogue number:

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Licensing provisions: none

Computer for which the program is designed and others on which it has been tested: CRAY C-90, SG Power Challenge L, IBM RS/6000

Operating systems: UNIX, UNICOS, IRIX, AIX

Programming language used: FORTRAN-77

Memory required to execute with typical data: 10 Mwords

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No. of bits in a word: 64

Has the code been vectorised?: Yes

No. of lines in distributed program: 19 438 (of which 8 354 are comments and separators)

Keywords: Hartree-Fock; Skyrme interaction; Self-consistent mean-field; Nuclear many-body problem; Superdeformation; Quadrupole deformation; Octupole deformation; Pairing; Nuclear radii; Single-particle spectra; Nuclear rotation; High-spin states; Moments of inertia; Level crossings; Harmonic oscillator; Coulomb field; Point symmetries

Nature of physical problem
The nuclear mean-field and an analysis of its symmetries in realistic cases are the main ingredients of a description of nuclear states. Within the Local Density Approximation, or for a zero-range velocity-dependent Skyrme interaction, the nuclear mean-field is local and velocity dependent. This allows an effective and fast solution of the self-consistent Hartree-Fock equations even for heavy nuclei and for different configurations, deformations, excitation energies, or angular momenta.

Method of solution
The program uses the Cartesian harmonic oscillator basis to expand single-particle wave functions of neutrons and protons interacting by means of the Skyrme effective interaction. The expansion coefficients are determined by the iterative diagonalization of the mean field Hamiltonians or Routhians which depend nonlinearly on the local neutron and proton densities. Suitable constraints are used to obtain states corresponding to a given configuration, deformation or angular momentum.

Restrictions on the complexity of the problem
The main restriction is the CPU time required for calculations of heavy deformed nuclei and for a given precision required. One symmetry plane is assumed. Pairing correlations are only included in the BCS limit and for the conserved time-reversal symmetry.

Typical running time
One Hartree-Fock iteration for the superdeformed, rotating, parity conserving state of $^{152}_{66}\text{Dy}_{86}$ takes about nine seconds on the CRAY C-90 computer. Starting from the Woods-Saxon wave functions, about fifty iterations are required to obtain the energy converged within the precision of about $0.1\,\text{keV}$. In case when every value of the angular velocity is converged separately, the complete superdeformed band with precisely determined dynamical moments $\mathcal{J}^{(2)}$ can be obtained within one hour of CPU on the CRAY C-90, or within two to three hours of CPU on the SG Power Challenge L or IBM RS/6000 computers. This time can be often reduced by a factor of three when a self-consistent solution for a given rotational frequency is used as a starting point for a neighboring rotational frequency.

Unusual features of the program

The user must have an access to the NAGLIB subroutine F02AXE or to the ESSL subroutine ZHPEV which diagonalize complex hermitian matrices, or provide another subroutine which can perform such a task.

The code is written in single-precision for the use on a 64-bit processor. The compiler option `-r8` or `+autodblpad` (or equivalent) has to be used to promote all real and complex single-precision floating-point items to double precision when the code is used on a 32-bit machine.

LONG WRITE UP

1 Introduction

The method of solving the Skyrme-Hartree-Fock (HF) equations in the Cartesian harmonic oscillator (HO) basis was described in the previous publication [1] which is referred to as I. The present paper is a long write up of the code HFODD which implements this method and solves the three-dimensional HF equations. A one-dimensional Skyrme-HF code restricted to the spherical symmetry has been published by P.-G. Reinhard [2]. Although several HF codes allowing triaxial deformations exist [3, 4, 5, 6], the code HFODD is the first one of that kind which is made available in the public domain. Several earlier beta versions of the code have already been distributed and used by various groups. The present version (v1.60n) is published for the first time and replaces all previous versions.

In Sec. 2 we present the numerical tests of the code, and in Secs. 3, 4, and 5 we describe its input, output, and source files, respectively.

2 Numerical tests

Accuracy of the solution of the HF equations with the wave functions expanded onto the Cartesian HO basis, Eq. (I-70),[3] depends on the three parameters $\hbar\omega_x$, $\hbar\omega_y$, $\hbar\omega_z$ defining the HO frequencies in three Cartesian directions, and on the number M of the HO states included in the basis. In the code HFODD we use the standard prescription [7, 8] to chose the HO states included in the basis, namely, the M states with the lowest HO single-particle energies,

$$\epsilon_{n_x n_y n_z} = \hbar\omega_x(n_x + \tfrac{1}{2}) + \hbar\omega_y(n_y + \tfrac{1}{2}) + \hbar\omega_z(n_z + \tfrac{1}{2}), \tag{1}$$

are selected among those which have $n_x \leq N_0$, $n_y \leq N_0$, and $n_z \leq N_0$, where N_0 is the fixed maximum number of HO quanta. It should be noted that in general both M and N_0 have to be specified to define the basis. Only for large N_0, the basis is defined solely by M and does not depend on N_0. In this case, the grid of points (n_x, n_y, n_z) defining the states included in the basis forms a pyramid in three dimensions, with the inclined face delimited by the condition $\epsilon_{n_x n_y n_z} \leq$ const. On the other hand, only for small values of N_0 the basis is defined solely by N_0 and does not depend on the energy cut-off. In this case the corresponding grid of points $n_x n_y n_z$ forms a cube of the size N_0. In all intermediate

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[3]Symbol (I-70) refers to Eq. (70) of I.

cases the shape of the basis corresponds to a pyramid with the corners cut off, or to a cube with the corners cut off. Usually N_0 is chosen large enough so that all the states allowed by the energy cut-off are included in the basis. The shape of the basis is printed in form of three projections by the code HFODD on the output file, see the TEST RUN OUTPUT below.

In what follows we discuss only the results obtained with axially deformed bases for $\omega_\perp = \omega_x = \omega_y$, and present the results in terms of the standard parameters

$$\omega_0 = (\omega_\perp^2 \omega_z)^{1/3} \quad \text{and} \quad q = \omega_\perp / \omega_z. \tag{2}$$

(The code accepts of course in general a triaxially deformed HO basis what offers the user some additional flexibility in approaching the actual physical problem). In Ref. [8] the dependence of results on the basis parameters and on the basis size has been tested for $N_0 \leq 10$, which at that time was at the limit of the numerical feasibility. In the present study we discuss similar tests up to $N_0 = 20$ (spherical case) and $N_0 = 26$ (deformed case).

From the tests based on low values of N_0, the authors of Ref. [8] concluded that the basis parameters ω_0 and q have to be optimized for a given basis size in such a way that the HF energy is minimized. This procedure is consistent with the variational character of the HF theory in which the best approximation to the energy is obtained by a minimization of the energy. Although the variational principle does not ensure that the best approximation to other observables is obtained for the wave functions corresponding to the minimum of energy, this turned out to be the case for low values of N_0. The necessity to optimize the basis parameters was the real bottleneck of the method, because it requires many HF calculations to be performed before one physical solution can been obtained.

The picture described above does not apply to calculations performed with relatively large values of N_0. Of course, the best energy is still obtained with optimized values of the basis parameters, but the energy depends now very weakly on the basis parameters and the error generated by using a non-optimal basis is small. Moreover, the best results for other observables are not necessarily obtained with the optimal basis parameters. This can be well understood by noticing that the minimum obtained from a very weak dependence of the energy on the basis parameters may be illconditioned, and may occur at rather accidental value. Therefore, for large values of N_0, the basis optimization does not bring any substantial improvement of precision. Instead of the optimization, suitable "physical" values of the basis parameters can be determined based on simple geometrical considerations. This is in line with results of Ref. [8], where it was shown that a partial optimization followed by the liquid-drop-model estimates reproduces the optimal basis parameters even for small values of N_0.

In the code HFODD the physical basis parameters are determined as follows (cf. also Ref. [3]). First we define ω_0 by the standard value [9] multiplied by some phenomenological factor f close to unity,

$$\hbar \omega_0 = f \times 41 \, \text{MeV}/A^{1/3}. \tag{3}$$

Based on the experience gained from the diagonalization of the Woods-Saxon Hamiltonian on the HO basis [10, 11], the recommended value is $f = 1.2$. This particular scaling of the oscillator frequencies turns out to help in stabilizing the results of the diagonalization

with respect to adding the new basis states. Second, suppose we wish to perform the HF calculations for a given set of multipole deformations $\alpha_{\lambda\mu}$, i.e., for a nuclear shape defined by the surface Σ

$$\Sigma: \ R(\theta, \phi) = c(\alpha) \left[1 + \sum_{\lambda=0}^{\lambda_{max}} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta, \phi) \right], \tag{4}$$

where $c(\alpha)$ is a function of $\alpha_{\lambda\mu}$ such that the volume enclosed by the surface Σ does not depend on α. Due to the assumed y-simplex symmetry, see Sec. 3.1 of I, all multipole deformations $\alpha_{\lambda\mu}$ are real, and only those with $\mu \geq 0$ are used in the code HFODD because then $\alpha_{\lambda,-\mu} = (-1)^\mu \alpha_{\lambda\mu}$.

The lengths of principal axes of the volume enclosed in the surface Σ can be defined as $R_x = R(\pi/2, 0)$, $R_y = R(\pi/2, \pi/2)$, and $R_z = R(0,0)$. For complicated shapes they do not necessarily correspond to the principal axes of the moment of inertia or quadrupole moment. However, when the quadrupole deformation dominates, this will roughly be so if the quadrupole deformation is considered in its intrinsic frame of reference, i.e., if one uses $\alpha_{21} = 0$. The relative values of the HO frequencies are then defined by the condition

$$\omega_x R_x = \omega_y R_y = \omega_z R_z, \tag{5}$$

while the common proportionality constant is given by the condition $(\omega_x \omega_y \omega_z)^{1/3} = \omega_0$.

The above prescription is very helpful if the values of physical deformations are (at least roughly) known for a given nucleus. This is true in particular for the superdeformed shapes which have very similar deformations in a given region of nuclei. For example, the superdeformed nuclei in the $A \sim 150$ region can be very well described in the basis corresponding to the ^{152}Dy nucleus with deformations $\alpha_{20} = 0.61$ and $\alpha_{40} = 0.10$ [12]. This gives the physical basis parameters, $\hbar\omega_x = \hbar\omega_y = 6.246$ MeV and $\hbar\omega_z = 11.200$ MeV, i.e., $\hbar\omega_0 = 9.219$ MeV and $q = 1.793$.

We may now present results of tests performed for different basis parameters and compare them with those obtained for the physical basis parameters. All calculations below have been performed for the Skyrme parametrization SkM* with the coupling constants $C_t^J = C_t^T = C_t^{\Delta s} = 0$ in the energy functional (I-12). The latter conditions correspond to simplifications of the Skyrme functional usually assumed in studies made within the spatial coordinates [13, 14], and allow a comparison of our results with those obtained by an independent method and an independent HF code.

From now on we are going to use the two adjectives introduced above and associated with the basis parameters: *optimal*, i.e., adjusted to a given basis size so as to minimize the HF energy, and *physical*, i.e., corresponding to the actual information about the deformations of nuclei studied, and calculated through Eqs. (3), (4), and (5) based on the experimental result or earlier Strutinsky-type calculations.

2.1 Spherical nuclei

We begin with the results obtained for a spherical nucleus ^{208}Pb for which the spherical basis is used, $q = 1$, and the results are studied in function of $\hbar\omega_0$. The physical value for this nucleus is $\hbar\omega_0 = 8.304$ MeV, and is represented in Figs. 1 and 2 by the vertical dashed

lines. The horizontal dashed lines represent very precise solutions obtained by the simple one-dimensional spherical code in spatial coordinates, and are considered as the exact values. The solid lines represent the results calculated by the code HFODD for N_0 from 10 to 18, and the asterisk represents the calculation with N_0=20. For the spherical bases the number of the HO states is given by $M=(N_0+1)(N_0+2)(N_0+3)/6$, and hence in Figs. 1 and 2 it increases from 286 to 1771.

The energies of ^{208}Pb, shown in Fig. 1, converge rather slowly to the exact value of -1635.956 MeV. For N_0=10 the error is about 6 MeV and only for $N_0 \geq 16$ becomes smaller than 1 MeV. For every value of N_0, the dot denotes the minimum of energy which defines the optimal value of $\hbar\omega_0$. For N_0=10 and 12 the optimal values are rather remote from the physical value and, moreover, two minima appear for N_0=12. For N_0=14 the minimum occurs at the physical value of $\hbar\omega_0$, but for larger bases, N_0=16 and 18, the minimum becomes poorly defined and deviates from the physical value of $\hbar\omega_0$.

Fig. 2 shows the corresponding results of calculations for the matter rms radii of ^{208}Pb. For every curve the dots represent the minima of the energies shown in Fig. 1. One should note that the vertical scale of the Figure is very much expanded and shows a narrow region of radii within about 0.3% around the exact value of R_{rms}=5.5546 fm. For N_0=10 the radii significantly depend on $\hbar\omega_0$ but the value of R_{rms} at the physical basis parameter is very close to the exact result, while the value at the optimal basis parameter is much worse. For N_0=12 the value at the physical $\hbar\omega_0$ is again much better than those at any of the two optimal bases. For N_0=14 the physical and optimal bases coincide and give the exact value with the error of 0.05%, while for larger bases the dependence of R_{rms} on $\hbar\omega_0$ becomes weak, and the results for the optimal bases are only slightly better than those for the physical basis. Altogether, for any value of $N_0 \geq 10$ the physical basis gives the radii precise up to ± 0.003 fm, or up to ± 0.05%.

2.2 Deformed nuclei

In order to study the properties of the optimization of the deformation of the basis, we have performed a series of calculations for the non-rotating superdeformed state in ^{152}Dy ($\hbar\omega$=0) with $\hbar\omega_0$ fixed at the physical value, and for several different values of q and M. These results can be compared to those obtained in spatial coordinates for the same nucleus and force, and with the three-dimensional cubic grid of points spaced by Δx=1.0, 0.8, or 0.7 fm. In this case smaller spacing gives more accurate results, and one obtains [15], respectively, the total energies $\mathcal{E}$=-1234.611, -1230.769, or -1230.104 MeV and the proton quadrupole moments Q_p=18.316, 18.369, or 18.376 b.

These values of energies were obtained by using the finite difference expressions for derivatives, which are less precise than the Fourier expressions [16]. If the HF equations are solved using the first type of approximation but nevertheless at the end of the convergence the energies are calculated with the second method, one obtains a good and cost-effective estimate of the energy [16, 17]. Such a procedure yields [15] for Δx=0.7 fm the value of $\mathcal{E}$=-1229.365 which we may consider for the purpose of the discussion below as the exact result. This energy is shown by the horizontal dashed line in Fig. 3. In practice, the three-dimensional calculations in the spatial coordinates are usually done with Δx=1 fm and employ the finite difference method. For these standard conditions the binding energy

of ^{152}Dy is overestimated by about 5 MeV.

Fig. 3 shows the total energies in ^{152}Dy calculated by the code HFODD for M=300, 600, 900, or 1200. When q varies from 1.3 to 2.3 the maximum numbers of the HO quanta in the directions perpendicular/parallel to the elongation axis vary for M=300 from 9/13 to 8/18 quanta. Similarly, for M=1200 and q=1.793 the HO basis contains 14/26 quanta. Here and in the following, the results for M=300 are presented as broken lines with visible jumps corresponding to individual states entering and leaving the HO basis. Indeed, keeping a fixed number M of states with varying q means that a given HO orbital may cross the boundary $\epsilon_{n_x n_y n_z} \leq$const. For relatively small values of M this may create some effects on various quantities (visible in the expanded scales of presented Figures), while for larger values of M such effects disappear.

The convergence of energy in function of M is again rather slow; for M=300 the error is around 5 MeV and it decreases to below 1 MeV only at M>600. For M=300 and 600 the optimal basis deformations are rather different from the physical value. However, the energy gain from optimizing the value of q is very small. For M=900 the optimal and physical values of q are close to one another, but the minimum of energy is hardly visible. For M=1200 we obtain $\mathcal{E}$=$-$1229.383 in a very good agreement with the exact result. I should be noted that both estimates compared here are variational, and hence both may still slightly decrease with further improvement of the numerical parameters.

Fig. 4 shows the values of proton quadrupole moments calculated by the code HFODD and compared with the value of 18.376 b obtained for Δx=0.7 fm (see above). The latter value is for the purpose of the present test considered as the exact result. Again the region shown on the ordinate is very narrow; within 0.5% of the value of Q_p. On the other hand, the region of q presented on the abscissa is fairly large; it corresponds to the standard quadrupole deformations $\beta \equiv \alpha_{20}$ of the nuclear surface (4) ranging from 0.3 to 1.0.

For M=300 one obtains much a better value of Q_p for the physical basis than for the optimal basis. This situation is reversed for M=600. For M=900 the dependence on basis parameters is very weak and the results are very close to the physical-basis value of Q_p=18.393 obtained for M=1200. The values of Q_p calculated by the code HFODD tend to be slightly larger than the exact value obtained within the spatial-coordinate method. We have checked that the optimization of $\hbar\omega_0$ does not remove this residual difference.

Similarly as for tests performed in spherical nuclei, one can conclude that the optimization of the basis does not, in general, improve the results as compared to those obtained for the physical basis. Within a very limited space of M=300 HO states one may obtain a very reasonable estimate of Q_p when the physical basis is used. Taking into account the fact that the discrepancy is larger for M=600, we may attribute a conservative error of 0.05 b, or 0.3% to the calculated values of the quadrupole moments. A precision of this order is perfectly sufficient for all practical purposes, and can of course be improved by using larger bases, instead of optimizing the basis parameters. In fact, the obtained precision is comparable to that of the spatial-coordinate method when it is used with the standard value of Δx=1 fm (see above).

2.3 Rotating nuclei

In Fig. 5 we show the values of the angular momentum I calculated for ^{152}Dy at $\hbar\omega=$ 0.5 MeV. For all values of q and M considered in the Figure one obtains results which are within $0.1\,\hbar$ of the value calculated for $M{=}1200$. Again, there is no advantage in using the optimal bases as compared to the physical one. The optimal values of q were obtained by minimizing the Routhian (I-21) at constant $\hbar\omega$. We do not show here the plot of the Routhian in function of q because such a plot is very similar to that of the energy at zero spin, Fig. 3, except for an almost constant shift by $-\omega I$.

The properties of superdeformed bands are very often described in terms of moments of inertia, which can be calculated as the static or dynamic (first or second) moments

$$\mathcal{J}^{(1)} = \frac{I}{\omega}, \tag{6a}$$

$$\mathcal{J}^{(2)} = \frac{dI}{d\omega}, \tag{6b}$$

respectively. The precision of determining $\mathcal{J}^{(1)}$ is therefore governed by that with which the total angular momentum I is calculated, and for $\hbar\omega{=}0.5$ MeV it is equal to about $0.2\,\hbar^2$/MeV. In practical calculations, the dynamic moment $\mathcal{J}^{(2)}$ has to be calculated by the finite-difference expression

$$\mathcal{J}^{(2)} = \frac{I(\omega_2) - I(\omega_1)}{\omega_2 - \omega_1} \tag{7}$$

which is precise up to

$$\delta\mathcal{J}^{(2)} \sim \tfrac{1}{24}(\omega_2 - \omega_1)^2 \frac{d^2\mathcal{J}^{(2)}}{d\omega^2}. \tag{8}$$

This expression for $\delta\mathcal{J}^{(2)}$ corresponds to the lowest-order term neglected in the Taylor expansion leading to the finite-difference formula (7). The curvature of $\mathcal{J}^{(2)}$, which determines its precision $\delta\mathcal{J}^{(2)}$, is usually fairly small (200–$300\,\hbar^4$/MeV^3 at most), except at the crossing frequencies where the precise values of $\mathcal{J}^{(2)}$ are physically not important anyhow. Therefore, the finite difference expression (7) can usually be used already at $\omega_2{-}\omega_1{\simeq}0.1$ MeV/$\hbar$.

In Fig. 6 we present results for $\mathcal{J}^{(2)}$ calculated at $\hbar\omega{=}0.55$ MeV by using the values of I obtained at $\omega_1{=}0.5$ and $\omega_2{=}0.6$ MeV/$\hbar$. In view of the precision of the total angular momentum I, estimated above to be equal to $0.1\,\hbar$, one could have expected that the values of $\mathcal{J}^{(2)}$ obtained in this way will be precise only up to about $1\,\hbar^2$/MeV. In fact, the real precision of $\mathcal{J}^{(2)}$ turns out to be an order of magnitude *better*. This is so because most of the errors related to the use of the finite HO basis cancel out, and the difference of angular momenta turns out to be much more precise that the total value of I itself. As a result, the dynamic moments $\mathcal{J}^{(2)}$ shown in Fig. 6 are precise up to $0.1\,\hbar^2$/MeV. This observation concerns also many other observables, and will be discussed in the next section in more detail.

2.4 Relative energies, moments, and alignments

As already pointed out in Ref. [8], the differences of energies (the relative energies) depend much less on the basis parameters than the total (absolute) energies. This is illustrated

in Fig. 7, where we show the proton separation energies S_p in the SD ^{152}Dy nucleus, calculated at spin zero for different values of q and M. The values of S_p have been calculated by subtracting the total energy of ^{152}Dy from the total energy of ^{151}Tb after both have been determined self-consistently by using the same HO basis. The SD state in ^{151}Tb has been constructed by creating a hole in the $\pi[651]3/2(+i)$ orbital, cf. Ref. [12]. As seen in the Figure, the separation energies are precise up to about $50\,$keV, which is two orders of magnitude better than the total energies in either of ^{151}Tb or ^{152}Dy nucleus. Similar precision is also expected for the excitation energies in a given nucleus, i.e., for the differences of energies corresponding to different configurations or angular momenta.

The same principle also works for the quadrupole polarizations [18] which are obtained by subtracting the quadrupole moments of the SD states in ^{151}Tb and ^{152}Dy nuclei. This is shown in Fig. 8, where the obtained quadrupole polarizations are precise up to $0.01\,$b, compared to the $0.05\,$b precision obtained for the values of proton quadrupole moments Q_p discussed above. Similarly, the relative alignments between these two nuclei, i.e., the differences of angular momenta at a given angular frequency, $\hbar\omega{=}0.5\,$MeV here, are presented in Fig. 9. These values characterize the quality of the identical bands [19], and have been discussed in Ref. [12]. Here we see that using the truncated HO basis they are precise up to $0.03\,\hbar$, which is a factor three better than the values of the angular momenta discussed in Sec. 2.3.

2.5 Summary

Table 1 summarizes the results discussed in Sections 2.1–2.4. The column denoted "absolute values" refers to the errors of observables calculated in ^{208}Pb or ^{152}Dy for $M{=}300$ and for the physical basis parameters. The errors are deduced by comparing these results with the exact ones, where available, or with the results obtained with $M{=}1200$. The percentage errors are also given. The column denoted "relative values" refers to the errors of differences of observables calculated in ^{151}Tb and ^{152}Dy. Due to the fact that most of the errors are systematic (they originate from the truncated HO basis), they tend to cancel out, and the errors of relative observables are smaller than those of the absolute observables. Since the relative values are much smaller than the absolute values, the percentage errors are larger in this case, but still only of the order of several per cent. In all cases the precisions of relative values are sufficient for a meaningful comparison with data or with other theories. Whenever more precise results are required, they can be easily obtained by increasing the size of the basis. The basis optimization is not a competing procedure which would lead to a better precision.

3   Input data file

Different aspects of the organization of the code HFODD are presented in this section together with the description of the input data file. The code reads the input data from the standard FORTRAN input file, prints results on the standard FORTRAN output file, and also writes two auxiliary files which below are called the review file and the record file. If required, the code may also start the iteration from the Woods-Saxon wave functions, which have to be provided in the specialized file called the Woods-Saxon file, or from the

previously recorded HF potentials provided in the file called the replay file.

The general structure of the input data file is defined by the following rules:

1. Input data file is an ASCII file composed of independent items.

2. An item is composed of the keyword line, and of the data line which follows immediately the keyword line. Two items contain no data lines, see point 6 below.

3. The keyword line contains in columns 1 through 10 a keyword which is a specific text defining the item. If the keyword has less than 10 characters it has to be obligatorily padded with appropriate number of trailing spaces. Columns beyond 10 are ignored and can be used to place arbitrary comments or texts.

4. The data line contains a prescribed number of data values which are read in the free FORTRAN FORMAT. The type of data (`REAL`, `INTEGER`, or `CHARACTER`) should match the definition of the given data line. The `CHARACTER` data should be provided starting from the 13-th column of the data line.

5. Items can be separated by an arbitrary numbers of comment lines. A line is treated as a comment and ignored provided it does not contain in columns 1 through 10 any of the valid keywords.

6. Two items contain no data lines. The first one is defined by the keyword `EXECUTE`, and starts a calculation for the currently defined input parameters. The second one is defined by the keyword `ALL_DONE`, and terminates the program. The latter item is not required if the compiler is able to properly recognize the end of input data file. When the end of input data file is encountered, the program terminates as if the keyword `ALL_DONE` was found.

7. A given item may occur any number of times in different places of the input data file. Only the last one of the same items occurring before a given `EXECUTE` keyword is taken into account.

8. Between two consecutive items `EXECUTE`, the order of other items is arbitrary. These other items define the data set, i.e, the set of input parameters, for which the calculation will start at the moment when the next item `EXECUTE` is found.

9. All input parameters have the default values defined in the code (subroutine PRE-DEF). Therefore, if the input data file contains only the item `EXECUTE`, and no other lines, a calculation for the default values will be performed. In the present version, this will result in performing 50 iterations for the superdeformed state of $^{152}_{66}\text{Dy}_{86}$ at the angular frequency of $\hbar\omega=0.5\,\text{MeV}$.

10. Only those items which define the values of input parameters which are different than the default values have to be included in the input data file. The values of input parameters defined by any item will stay in effect till another occurrence of the same item, or till the code terminates. This rule is valid irrespectively of how many `EXECUTE` items follow the given item.

Together with the FORTRAN source code in the file `hfodd.f`, two input data files are provided, `dy152-a.dat` and `dy152-b.dat`. The first one contains only one line with the keyword `EXECUTE`. The second one, which is reproduced in the section TEST RUN INPUT below, contains all valid keywords and the input parameters identical to the default values. Therefore, the results of executing the program for the both provided input data files are strictly identical. The second input data file serves only as a suitable pattern to modify the input parameters. However, it should be a good practice to include in the input data file only those items which modify the input parameters with respect to the default values. In this way, a danger of accidentally modifying some intricate numerical parameters of the code is minimized.

In the following subsections we discuss all the valid keywords and their corresponding data lines. The default values are given in the data lines following the keyword lines. In the data lines we also show names of the corresponding variables which are referred to in the text. The meaning of several parameters that are introduced below in the context of their function in the code is explained in detail in I.

3.1   General data

Keyword: `NUCLID`
$$86, 66 = \text{IN\_FIX}, \text{IZ\_FIX}$$
Numbers of neutrons (`IN_FIX`) and protons (`IZ_FIX`) in the nucleus under consideration. Calculations for odd and odd-odd nuclei require `IROTAT=1`.

Keyword: `ITERATIONS`
$$50 = \text{NOITER}$$
For `NOITER`>0, the specified number of iterations is performed. The code starts with the iteration number 0 by constructing the initial potentials. Specifying `NOITER=0` requests only this initial phase. If the iteration is restarted from the previously recorded potentials (`ICONTI=1`), then the counting of iterations continues from the previous value on.

3.2   Interaction

Keyword: `SKYRME-SET`
$$\text{SKM* = SKYRME}$$
`CHARACTER*4` acronym of the Skyrme force parameter set. Must start at the 13-th column of the data line. At present, valid acronyms are SKM*, SIII, SKP, and SKI1. Other sets of parameters can easily be included in the subroutine PARAMS.

Keyword: `EVE_SCA_TS`
$$1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.$$
                    SRHO_T, SRHO_S, SRHODT, SRHODS, SLPR_T, SLPR_S,
                                        STAU_T, STAU_S,
                                        SSCU_T, SSCU_S,
                                        SDIV_T, SDIV_S
By using this item in the data set the coupling constants corresponding to a given Skyrme parameter set can be arbitrarily scaled. This allows calculations with modified Skyrme

functionals [12]. The time-even coupling constants in the total-sum representation (I-14) are multiplied by the 12 numbers from `SRHO_T` to `SDIV_S`. The variables with names ending with `_T` and `_S` multiply the "total" and "sum" coupling constants, respectively. The variables with names containing the acronyms `RHO`, `LPR`, `TAU`, `SCU`, and `DIV`, multiply the coupling constants with superscripts ρ, $\Delta\rho$, τ, J, and ∇J, respectively, and those with `RHOD` multiply the density-dependent part of C^ρ. Similar name convention is used for many other variables in the code HFODD.

Keyword: `ODD_SCA_TS`

$$1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.$$

```
                    SSPI_T, SSPI_S,SSPIDT, SSPIDS,SLPS_T, SLPS_S,
                                            SCUR_T, SCUR_S,
                                            SKIS_T, SKIS_S,
                                            SROT_T, SROT_S
```

Same as above but for the time-odd coupling constants. Acronyms `SPI`, `LPS`, `CUR`, `KIS`, and `ROT` correspond to coupling constants with superscripts s, Δs, T, j, and ∇j, respectively, and those with `SPID` correspond to the density-dependent part of C^s.

Keyword: `EVE_SCA_PM`

$$1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.$$

```
                    SRHO_P, SRHO_M,SRHODP, SRHODM,SLPR_P, SLPR_M,
                                            STAU_P, STAU_M,
                                            SSCU_P, SSCU_M,
                                            SDIV_P, SDIV_M
```

Same as above but for the time-even coupling constants in the isoscalar-isovector representation, Eq. (I-15). The variables with names ending with `_P` and `_M` multiply the isoscalar and isovector coupling constants, respectively. The total-sum scaling factors are used first, and the isoscalar-isovector scaling factors are used afterwards.

Keyword: `ODD_SCA_PM`

$$1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.$$

```
                    SSPI_P, SSPI_M,SSPIDP, SSPIDM,SLPS_P, SLPS_M,
                                            SCUR_P, SCUR_M,
                                            SKIS_P, SKIS_M,
                                            SROT_P, SROT_M
```

Same as above but for the time-odd coupling constants in the isoscalar-isovector representation, Eq. (I-15).

Keyword: `G_SCALING`

$$1.0, 1.0 = \texttt{FACTGN, FACTGP}$$

For `IPAIRI=1` the code HFODD solves the BCS equations with the neutron and proton pairing strengths defined in Ref. [20]. These values can be modified by defining here the multiplicative factors `FACTGN` and `FACTGP` for neutrons and protons, respectively.

3.3 Symmetries

Keyword: `ROTATION`

$$1 = \texttt{IROTAT}$$

Calculation with time-reversal breaking will be performed for `IROTAT`=1, while the time-reversal symmetry will be conserved for `IROTAT`=0. In the latter case the calculations will be performed only for one value of the simplex, $s=+i$, which gives almost twice shorter execution times. `IROTAT`=0 is incompatible with providing a non-zero value of the angular frequency or with attempting a calculation for an odd or odd-odd nucleus.

Keyword: `SIGNATUREY`

$$1 = \texttt{ISIGNY}$$

Calculation with parity/signature symmetry conserved are performed for `ISIGNY`=1, while the parity (and signature) will be broken for `ISIGNY`=0. In the former case the parity blocks will be separately diagonalized and the densities will be summed only in the 1/8 of all the Gauss-Hermite nodes. This may give almost twice shorter execution times. `ISIGNY`=1 requires `ISIMTX`=`ISIMTZ`=1, and `ISIGNY`=0 requires `ISIMTX`=0, or `ISIMTZ`=0, or `ISIMTX`=`ISIMTZ`=0, see Sec. 3.4 of I.

Keyword: `TSIMPLEXES`

$$1, 1 = \texttt{ISIMTX, ISIMTZ}$$

Calculation with conserved symmetries given by x-simplex^T and/or z-simplex^T, see Sec. 3.4 of I, will be performed for `ISIMTX`=1 and/or `ISIMTZ`=1, respectively. These symmetries will be broken for `ISIMTX`=0 and `ISIMTZ`=0. Values of `ISIMTX` and `ISIMTZ` should be compatible with that of `ISIGNY` in such a way that `ISIGNY`=`ISIMTX`*`ISIMTZ`.

Keyword: `PAIRING`

$$0 = \texttt{IPAIRI}$$

Calculation without pairing correlations (pure HF) will be performed for `IPAIRI`=0 while the BCS pairing correlations will be included for `IPAIRI`=1. The latter case is incompatible with `IROTAT`=1.

3.4 Configurations

Keyword: `VACSIM_NEU`

$$43, 43 = \texttt{KVASIM(0), KVASIM(1)}$$

Numbers of lowest neutron states occupied in the two blocks, denoted by $(+)$ and $(-)$, of given simplexes, $s=+i$ and $s=-i$, respectively. These numbers define the simplex reference configuration from which the particle-hole excitations are counted. The definitions of simplex reference configuration and excitations are ignored unless `ISIGNY`=0 and `IPAIRI`=0.

Keyword: `VACSIM_PRO`

$$33, 33 = \texttt{KVASIM(0), KVASIM(1)}$$

Same as above but for the numbers of proton states.

Keyword: `PHSIMP_NEU`

$$1, 00, 00, 00, 00 = \texttt{NUPAHO, KPSIMP, KPSIMM, KHSIMP, KHSIMM}$$

Neutron particle-hole excitations in the simplex blocks. `NUPAHO` is the consecutive number from 1 to 5 (up to five sets of excitations can be specified in separate items). Particles are removed from the `KHSIMP`-th state in the $(+)$ block and from the `KHSIMM`-th state in the $(-)$ block, and put in the `KPSIMP`-th state in the $(+)$ block and in the `KPSIMM`-th

state in the $(-)$ block. At every stage of constructing excitations the Pauli exclusion principle has to be respected (particle removed from an occupied state and put in an empty state). Values equal zero have no effect. In practice, reasonable excitations can only be constructed by consulting the printed lists of single-particle states with their consecutive numbers in given blocks, see the TEST RUN OUTPUT below.

Keyword: `PHSIMP_PRO`

$$1, 00, 00, 00, 00 = \text{NUPAHO, KPSIMP, KPSIMM, KHSIMP, KHSIMM}$$

Same as above but for the proton particle-hole excitations.

Keyword: `VACSIG_NEU`

$$22, 22, 21, 21 = \text{KVASIG(0,0), KVASIG(0,1),}$$
$$\text{KVASIG(1,0), KVASIG(1,1)}$$

Numbers of lowest neutron states occupied in the four blocks, denoted by $(+,+)$, $(+,-)$, $(-,+)$, and $(-,-)$, of given (parity,signature) combinations, i.e., $(\pi, r)=(+1,+i)$, $(+1,-i)$, $(-1,+i)$, and $(-1,-i)$, respectively. These numbers define the parity/signature reference configuration from which the particle-hole excitations are counted. The definitions of parity/signature reference configuration and excitations are ignored unless `ISIGNY`=1 and `IPAIRI`=0.

Keyword: `VACSIG_PRO`

$$16, 16, 17, 17 = \text{KVASIG(0,0), KVASIG(0,1),}$$
$$\text{KVASIG(1,0), KVASIG(1,1)}$$

Same as above but for the numbers of proton states.

Keyword: `PHSIGN_NEU`

$$1, 00,00,00,00, 00,00,00,00 = \text{NUPAHO,}$$
$$\text{KPPPSP, KPPPSM, KPPMSP, KPPMSM,}$$
$$\text{KHPPSP, KHPPSM, KHPMSP, KHPMSM}$$

Neutron particle-hole excitations in the parity/signature blocks. Basic principles are the same as for the excitations in the simplex blocks. Particles are removed from the `KHPPSP`-th state in the $(+,+)$ block, from the `KHPPSM`-th state in the $(+,-)$ block, from the `KHPMSP`-th state in the $(-,+)$ block, and from the `KHPMSM`-th state in the $(-,-)$ block, and put in the `KPPPSP`-th state in the $(+,+)$ block, in the `KPPPSM`-th state in the $(+,-)$ block, in the `KPPMSP`-th state in the $(-,+)$ block, and in the `KPPMSM`-th state in the $(-,-)$ block.

Keyword: `PHSIGN_PRO`

$$1, 00,00,00,00, 00,00,00,00 = \text{NUPAHO,}$$
$$\text{KPPPSP, KPPPSM, KPPMSP, KPPMSM,}$$
$$\text{KHPPSP, KHPPSM, KHPMSP, KHPMSM}$$

Same as above but for the proton particle-hole excitations.

3.5 Ensemble of specific parameters referred to as "Numerical data"

Keyword: `MAX_MULTIP`

$$2, 4, 4 = \text{NMUCON, NMUCOU, NMUPRI}$$

Maximum multipolarities λ of multipole moments used in the code for the constraints, Eq. (I-22), surface term of the Coulomb field, Eq. (I-101), and printed on the output,

respectively. Values not larger than $\lambda=9$ are currently allowed. In case of the conserved parity/signature, only even multipoles are used in the Coulomb field.

Keyword: `COULOMB`

$$80,\ 79,\ 0.25 = \texttt{NUMCOU},\ \texttt{NUMETA},\ \texttt{FURMAX}$$

`NUMCOU` gives the number of points N^{Coul}, Eq. (I-100), used when summing up the Coulomb Green function. The dimensionless parameter d defining the size of the Coulomb parallelepiped, Eqs. (I-102) and (I-96), is given by `NUMCOU*FURMAX`. `NUMETA` gives the order of the Simpson integration of the solid harmonics on the faces of the parallelepiped, see Sec. 5 of I.

Keyword: `SLOW-DOWN`

$$0.5,\ 0.5 = \texttt{SLOWEV},\ \texttt{SLOWOD}$$

The standard prescription to calculate the HF potential in the next iteration is to mix a given fraction ϵ of the HF potentials from the previous iteration, with the fraction $1-\epsilon$ of potentials given by expressions (I-27). `SLOWEV` and `SLOWOD` give the values of ϵ separately for the time-even and time-odd potentials.

Keyword: `EPS_HERMIT`

$$1.0\mathrm{E}{-}14 = \texttt{EPSHER}$$

Numerical precision requested for determining values of Hermite polynomials.

Keyword: `OPTI_GAUSS`

$$1 = \texttt{IOPTGS}$$

For `IOPTGS=1` and `IREAWS=0`, expression (I-94) is used to calculate the order of the Gauss-Hermite integration, and the input parameters `NXHERM`, `NYHERM`, and `NZHERM` are ignored.

Keyword: `GAUSHERMIT`

$$18,\ 18,\ 32 = \texttt{NXHERM},\ \texttt{NYHERM},\ \texttt{NZHERM}$$

Orders L_x, L_y, and L_z of the Gauss-Hermite integration in three Cartesian directions. Must be even. Ignored if `IOPTGS=0` or `IREAWS=1`.

3.6 Parameters of the HO basis

Keyword: `BASIS_SIZE`

$$15,\ 301,\ 800.0 = \texttt{NOSCIL},\ \texttt{NLIMIT},\ \texttt{ENECUT}$$

The HO basis is composed of states having not more than $N_0=$`NOSCIL` quanta in either of the Cartesian directions, and not more than $M=$`NLIMIT` states in total, see Sec. 2. The states are added to the basis according to the increasing energy of the deformed harmonic oscillator (1). In case of degenerate HO states (e.g., for an axially deformed HO) the complete multiplets are included, so the actual number of states `LDBASE` can be slightly larger than `NLIMIT`. If `NLIMIT>0`, the cut-off energy `ENECUT` is ignored; otherwise all states having HO energy smaller then `ENECUT` are included in the basis, and `NLIMIT` is ignored.

Keyword: `HOMEGAZERO`

$$1.2 = \texttt{FCHOMO}$$

The code uses the standard value of the spherical HO frequency $\hbar\omega_0=41\,\mathrm{MeV}/A^{1/3}$ multiplied by the scaling factor $f=$`FCHOMO`, see Eq. (3).

Keyword: `SURFAC_PAR`

$$86, 66, 1.23 = \texttt{INNUMB, IZNUMB, ROPARM}$$

The code HFODD calculates parameters of the HO basis, and the zero-iteration Nilsson potential, by defining the standard classical surface Σ, Eq. (4), corresponding to the volume $\frac{4}{3}\pi * \texttt{ROPARM}^3 * (\texttt{INNUMB+IZNUMB})$.

Keyword: `SURFAC_DEF`

$$2, 0, 0.61 = \texttt{LAMBDA, MIU, ALPHAR}$$

The code defines frequencies of the deformed HO in three directions by using relation (5), $\omega_x R_x = \omega_y R_y = \omega_z R_z$, where R_μ are the lengths of principal axes of the nuclear surface Σ defined in the standard way (4) by real deformation parameters $\alpha_{\lambda\mu} = \texttt{ALPHAR(LAMBDA,MIU)}$. The overall factor is defined by $(\omega_x \omega_y \omega_z)^{1/3} = \omega_0$. For details see Sec. 2.

3.7 Constraints

Keyword: `OMEGAY`

$$0.5 = \texttt{OMEGAY}$$

Value of the cranking rotational frequency $\omega_J = \texttt{OMEGAY}$, Eqs. (I-23) and (I-24). Non-zero value requires `IROTAT=1`. Pure linear constraint on the value of spin, $\omega_y = \omega_J$ is used for `IFLAGI=0`.

Keyword: `MULTCONSTR`

$$2, 0, 0.01, 42.0, 1 = \texttt{LAMBDA, MIU, STIFFQ, QASKED, IFLAGQ}$$

For `IFLAGQ=1`, the mass multipole moment of the given multipolarity λ and μ is constrained. Values of `LAMBDA`, `MIU`, `STIFFQ`, and `QASKED` correspond respectively to λ, μ, $C_{\lambda\mu}$, and $\bar{Q}_{\lambda\mu}$ in Eq. (I-22). For `IFLAGQ=0`, there is no constraint in the given multipolarity.

Keyword: `SPINCONSTR`

$$0.0, 0.0, 0 = \texttt{STIFFI, ASKEDI, IFLAGI}$$

For `IFLAGI=1`, the quadratic constraint on spin is used together with the linear constraint. Values of `STIFFI` and `ASKEDI` correspond respectively to C_J and $\bar{J}_y$ in Eq. (I-23). For `IFLAGI=0`, there is no quadratic constraint on spin, (but there still can be the standard cranking linear constraint defined by `OMEGAY`).

3.8 Output-file parameters

Keyword: `PRINT-ITER`

$$1, 0, 1 = \texttt{IPRSTA, IPRMID, IPRSTO}$$

The code prints results for the first, middle, and/or last iteration if the corresponding parameters `IPRSTA`, `IPRMID`, and `IPRSTO` equal 1.

Keyword: `EALLMINMAX`

$$-12.0, 0.0 = \texttt{EMINAL, EMAXAL}$$

The code prints tables of single-particle properties for states with values of the single-particle Routhians between `EMINAL` and `EMAXAL`. No table is printed unless `EMINAL` $\leq$ `EMAXAL`.

3.9 Files

Keyword: `REVIEWFILE`
$$\text{HFODD.REV} = \text{FILREV}$$
`CHARACTER*68` file name of the review file. Must start at the 13-th column of the data line. The ASCII review file is written after calculating every data set (i.e., once per every `EXECUTE` item), provided `IREVIE`>0. The file is not rewound, so the results for several data sets can be accumulated in a single file. This is so provided the filename `FILREV` is not changed between the `EXECUTE` items. The file contains all relevant parameters and results of calculation in a form suitable for reading by another program. It is ment as an interface to programs which analyze and/or plot the results. The file contains sections defined by keywords (different than keywords used in the input data file described here). The detailed structure of the review file is not documented in the present write up, and can be inferred from inspecting the specimen produced by the sample run, and from the subroutine REVIEW.

Keyword: `REVIEW`
$$2 = \text{IREVIE}$$
The review file will not be written if `IREVIE`=0. For `IREVIE`=2, the table of single-particle properties is included in the review file in addition to other results which are written for `IREVIE`=1.

Keyword: `RECORDFILE`
$$\text{HFODD.REC} = \text{FILREC}$$
`CHARACTER*68` file name of the record file. Must start at the 13-th column of the data line. The binary record file is written after each HF iteration. It contains complete information which allows restarting the iteration in another run of the code. To restart, one has to specify `ICONTI`=1 and provide the name of the file by defining `FILREP`. In case of the computer crush, the record file contains the results of the last performed iteration. Upon a successful completion of the given input data set it contains the results of the last performed iteration. The file is always rewound before it is written, so the results for consecutive iterations do not pile up.

Keyword: `REPLAYFILE`
$$\text{HFODD.REP} = \text{FILREP}$$
`CHARACTER*68` file name of the replay file. Must start at the 13-th column of the data line. The binary replay file with the name defined in `FILREP` must exist if `ICONTI`=1, and will be read. If the filenames `FILREP` and `FILREC` are identical, the replay file will be subsequently overwritten as a new record file. These feature is implemented to facilitate chaining of jobs which follow one another.

Keyword: `WOODSAFILE`
$$\text{WOODS.WFN} = \text{FILWOO}$$
`CHARACTER*68` file name of the Woods-Saxon file. Must start at the 13-th column of the data line. This file is read provided `IREAWS`=1. The binary Woods-Saxon file constitutes an interface between the Woods-Saxon code and the code HFODD. It contains the Woods-Saxon wave functions and numerous other parameters which define the current calculation.

The parameters read from the Woods-Saxon file overwrite the values provided in the input data file. Since the current version of the Woods-Saxon code will be published separately [21], the feature of starting the iteration from the Woods-Saxon results is not documented in the present write up.

3.10   Starting the iteration

Keyword: `RESTART`
$$0 = \texttt{ICONTI}$$
For `ICONTI=1`, results stored in the replay file (written as a record file in a previous run) will be used to start the iteration. The replay file name should be provided by defining `FILREP`. If the previous run was done with `IREAWS=1`, the current run must also use `IREAWS=1`, and the same Woods-Saxon file must be provided. This so because the Woods-Saxon file contains not only the information about the starting potential (which is ignored for `ICONTI=1`) but also defines the HO basis.

Keyword: `READ_WOODS`
$$0 = \texttt{IREAWS}$$
For `IREAWS=1`, the results stored by the previously performed Woods-Saxon calculation will be used to start the iteration and to define the HO basis. For `ICONTI=1` and `IREAWS=1` the Woods-Saxon file must also be provided, and will be used only to define the HO basis.

Keyword: `NILSSONPAR`
$$0, -1.175, -0.247, -1.175, -0.352, 11.17, 11.17, 6.28 =$$
$$\texttt{NILDAT, CNILSN, DNILSN, CNILSP, DNILSP,}$$
$$\texttt{HBANIX, HBANIY, HBANIZ}$$
For `IREAWS=0` and `ICONTI=0`, the code starts the calculation from the Nilsson potential. If `NILDAT=1`, the Nilsson parameters C and D [Ref. [22], Eq. (2.89)] are for neutrons given by `CNILSN` and `DNILSN` and for protons by `CNILSP` and `DNILSP`, while the HO deformation is defined by `HBANIX`, `HBANIY`, and `HBANIZ`. If `NILDAT=0`, the Nilsson parameters C and D are defined by Eq. (2.91) and Table 2.3 of Ref. [22], while the HO deformation is the same as that of the HO basis defined in Sec. 3.6. In the latter case the Nilsson parameters read from the input file are ignored.

4   Output file

Together with the FORTRAN source code in the file `hfodd.f`, an example of the output file is provided in `dy152.out`. Selected lines from this file are presented in the section TEST RUN OUTPUT below. This output file corresponds to the input file `dy152-b.dat` reproduced in the section TEST RUN INPUT below. Most of the information printed on the output file is self-explanatory. Here we only give some details which are not explicit in the output file.

The output file begins with the information pertaining to the general parameters of the calculation, then gives information about the starting point of the iteration, provides the convergence report, and finally contains the results calculated at the last iteration.

Section `CLASSICAL NUCLEAR SURFACE` lists the deformation parameters used to define the nuclear surface, Eq. (4), from which the basis parameters are derived, as described in Sec. 2. It also gives the basis parameters such as the `OSCILLATOR FREQUENCIES`: `HBAROX`, `HBAROY`, and `HBAROZ` corresponding to $\hbar\omega_x$, $\hbar\omega_y$, and $\hbar\omega_z$.

Section `PHYSICAL CONSTANTS` gives the values of $\hbar c$ in MeV fm (`H_BARC`), of $\hbar c/e^2$ (`HBCOE2`), of the neutron and proton masses in MeV$/c^2$ (`XMASSN` and `XMASSP`), of the kinetic-energy coefficient $\hbar^2/2m$ before (`HBMASS`) and after the center-of-mass correction (`HBMRPA`), Eq. (I-10), of the elementary charge squared e^2 in MeV fm (`ECHAR2`), and of the coefficient preceding the integral in the Coulomb exchange energy (`COULEX`), Eq. (I-19). For details see the comments in the SETBAS subroutine.

Section `OSCILLATOR LENGTHS`, `CONSTANTS`, and `FREQUENCIES` gives the values of $1/b_\mu$, b_μ, and $\hbar\omega_\mu$, respectively, which characterize the HO basis in three Cartesian directions, $\mu=x$, y, z.

Section `BASIS CUT-OFF CONTROL PARAMETERS` gives maximum numbers of the HO quanta in three directions `NXMAXX`, `NYMAXX`, and `NZMAXX` corresponding to N_x, N_y, and N_z, Eq. (I-70), as well as the orders of the Gauss-Hermite quadratures `NXHERM`, `NYHERM`, and `NZHERM`, corresponding to L_x, L_y, and L_z, Eq. (I-92). It also gives the number M of the HO states included in the basis as requested in the input file (`NLIMIT`) and as used in the calculation (`LDBASE`).

Section `SHAPE OF THE OSCILLATOR-BASIS DIAMOND` gives the numbers of the HO quanta in a given direction for fixed numbers of the HO quanta in both remaining directions. The output is arranged in such a way that the shape of the grid of points $n_x n_y n_z$ is clearly visualized by projections in every of the three directions.

Section `PARAMETER SET` gives the name and the values of the Skyrme force parameters, while the following section `COEFFICIENTS DEFINING THE SKYRME FUNCTIONAL` gives the corresponding values of the coupling constants in the Skyrme functional (I-12). These values take into account the scaling factors, Sec. 3.2, which are printed in the section `SCALING FACTORS` unless all are equal 1.

Sections `PARITY/SIGNATURE CONFIGURATIONS` or `SIMPLEX CONFIGURATIONS` give the vacuum and particle-hole configurations requested in the input file for the case of the parity symmetry conserved or not conserved, respectively.

Section `CONVERGENCE REPORT` gives the list of performed iterations. For each iteration one line is printed with the energy (I-9), stability (I-37), average values of the quadrupole moments Q_{20} and Q_{22}, total angular momentum, angular frequency (I-24), and the ratio of energies $\mathcal{E}/\tilde{\mathcal{E}}$, see Sec. 2.5 of I. The line corresponding to the last iteration is not printed because a more detailed information is given for the final state below this section.

Section `SINGLE-PARTICLE PROPERTIES` lists the single-particle states calculated for the Nilsson, Woods-Saxon, or Hartree-Fock Routhian operators. For every state one line is printed which gives the value of the single-particle Routhian, cf. Eq. (31), the consecutive numbers in the parity/signature or simplex blocks, the quantum numbers $[N, n_z, \Lambda]\Omega$ of the asymptotic Nilsson state which has the largest component in the given state, the average value of the parity operator (in %), the average values of projections of the intrinsic and total angular momenta (in $\hbar$), and their ratio called the g-factor.

Sections `MULTIPOLE MOMENTS` give the values of neutron, proton, or mass multipole moments in units of $(10\,\text{fm})^\lambda$. Traditional normalization factors are used as explained in

the comments in the subroutine DEFUNI. In particular, the $\lambda=0$ moment corresponds to the number of particles.

Sections ROOT-MEAN-SQUARE AND GEOMETRIC SIZES gives the rms average values of the radius and of the x, y, and z coordinates. In order to better visualize the size of the nucleus, the geometric sizes are also calculated by multiplying the rms radius by $\sqrt{5/3}$ and the rms coordinates by $\sqrt{5}$.

Section DENSITY INTEGRALS IN THE SKYRME FUNCTIONAL gives the integrals of products of densities, which appear in the Skyrme functional (I-12). The terms in the functional are identified by the acronyms described in Sec. 3.2.

Section CONTRIBUTIONS TO ENERGY IN THE SKYRME FUNCTIONAL gives the values of various terms which appear in the Skyrme functional (I-12). These contributions are the products of the coupling constants and of the density integrals described above. The sums of time-even and time-odd contributions are also printed.

Section ANGULAR MOMENTA gives the average values of the total and intrinsic neutron, proton, and total angular momentum (in $\hbar$). It also gives the corresponding values and contributions to the first moment of inertia $\mathcal{J}^{(1)}{=}I/\omega$ (in $\hbar^2/\mathrm{MeV}$).

Sections NEUTRON CONFIGURATIONS and PROTON CONFIGURATIONS give a visual representation of states occupied in the parity/signature or simplex blocks. The lines denoted by CONF: give the configurations requested in the input data set, while those denoted by VACC: give the configurations characterizing the given HF state. By comparing the two sets one can verify whether the requested configuration has been obtained, and eventually devise a new configuration to be calculated. The consecutive numbers printed in the horizontal direction correspond to the consecutive numbers in blocks printed in the section SINGLE-PARTICLE PROPERTIES. By comparing the two sections one can effectively associate the Nilsson labels with the calculated configurations and also prepare the configuration input data described in Sec. 3.4.

Section ENERGIES gives a summary of the energies calculated for the HF state. The kinetic (I-10), single-particle (I-32), and pairing (I-20) energies are printed for neutrons (NEU), protons (PRO), and all particles (TOT). The direct (DIR) and exchange (EXC) Coulomb energies, Eqs. (I-17a) and (I-19), are printed together with their sum (TOT). The multipole (MULT) and cranking (SPIN) constraint energies, Eqs. (I-22) and (I-23), are printed together with the corresponding corrections (CORR.) given by Eqs. (I-35) and (I-36), respectively. Then the rearrangement energy (I-34) is printed followed by the value of the Routhian (I-21) and the spin-orbit and Skyrme energies, the latter two split in the time-even (EVE) and time-odd (ODD) contributions. Finally, the total energies $\tilde{\mathcal{E}}$ (I-33) and $\mathcal{E}$ (I-9) are printed as (SP) and (FUN), respectively, while their difference (I-37) is printed as the stability (STAB).

5   FORTRAN source file

The FORTRAN source code in is provided in the file hfodd.f and can be modified in several places which are described in this section.

5.1 Dimensions of arrays

The code HFODD uses the arrays' dimensions declared through the `PARAMETER` statements. This allows changing the dimensions and adapting the size of the reserved memory to the problem being solved. Whenever too small a dimension is defined the code aborts with a message indicating the dimension which should be increased. Substantial amount of memory is required only for arrays depending on the following `PARAMETER` values:

`PARAMETER (NDMAIN=16)`
Should be larger or equal to the input parameter `NOSCIL` defined in Sec. 3.6.

`PARAMETER (NDBASE=307)`
Should be larger or equal to the input parameter `NLIMIT` defined in Sec. 3.6. It should also be larger or equal to the actual size of the HO basis `LDBASE`, which can be larger than `NLIMIT` in case of degenerate HO states.

`PARAMETER (NDXHRM=19,NDYHRM=19,NDZHRM=33)`
Should be respectively larger or equal to the input parameters `NXHERM`, `NYHERM`, and `NZHERM` defined in Sec. 3.5.

On vector machines, parameters `NDXHRM`, `NDYHRM`, `NDZHRM`, and `NDBASE` should be odd in order to minimize the risk of bank memory conflicts. By the same token, parameter `NDMAIN` should be even, because it defines the matrix dimensions beginning with 0.

5.2 Vectorization properties

As discussed in Sec 4.3 of I, the code HFODD has to operate by using seven-fold nested short loops, and this part does not perform well in a vector processor. However, it turns out that the loops can be artificially made longer in such a way that the final CPU time in a vector processor actually becomes much shorter. All the places where this trick has been applied can be identified in the source file by finding the lines beginning with `CVECTOR` and `CSCALAR`, for example:

```
CVECTOR
                   DO KZ=0,LAZOXY(NX,NY)+LAZOXY(MX,MY)
CSCALAR            DO KZ=NZ+MZ,0,-2
                      RESULT=RESULT+COEF00(KZ,NZ,MZ,3)*T_AUXI(KZ)
                   END DO
```

The line beginning with `CSCALAR` should be made active on a scalar or superscalar machine. The line immediately below the line which begins with `CVECTOR` should be active on a vector machine. The results of calculation do not depend on which version of loops is activated.

5.3 Library subroutines

The code HFODD requires an external subroutine which diagonalizes complex hermitian matrices. In the present version, the code calls the NAGLIB subroutine F02AXE. The call to this subroutine is performed through the interface subroutine ZHPEV, which can be replaced by the ESSL subroutine of the same name and the same calling parameters.

In the present version, the code also uses an external subroutine CGEMM from the BLAS CRAY library, which multiplies three complex matrices. By using the value of PARAMETER (I_CRAY=0) the call is diverted to the functionally equivalent subroutine ZGEMUL, which is provided in the source file. However, the latter one can also be replaced by the ESSL subroutine of the same name and the same calling parameters.

6 Acknowledgments

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TEST RUN INPUT

```
                         ----------  General data  ----------
NUCLID
            86    66
ITERATIONS
            50
                         ----------  Interaction  -----------
SKYRME-SET
            SKM*
EVE_SCA_TS   RHO       RHOD      LPR       TAU       SCU       DIV
            1.  1.    1.  1.    1.  1.    1.  1.    1.  1.    1.  1.
ODD_SCA_TS   SPI       SPID      LPS       CUR       KIS       ROT
            1.  1.    1.  1.    1.  1.    1.  1.    1.  1.    1.  1.
EVE_SCA_PM   RHO       RHOD      LPR       TAU       SCU       DIV
            1.  1.    1.  1.    1.  1.    1.  1.    1.  1.    1.  1.
ODD_SCA_PM   SPI       SPID      LPS       CUR       KIS       ROT
            1.  1.    1.  1.    1.  1.    1.  1.    1.  1.    1.  1.
G_SCALING
            1.0  1.0
                         ----------  Symmetries  ------------
ROTATION
            1
SIGNATUREY
            1
TSIMPLEXES
            1      1
PAIRING
            0
                         ----------  Configurations  --------
VACSIM_NEU       SIMP  SIMM
                 43    43
VACSIM_PRO       SIMP  SIMM
                 33    33
PHSIMP_NEU        PART              HOLE
            1    00    00        00    00
PHSIMP_PRO        PART              HOLE
            1    00    00        00    00
VACSIG_NEU   PPSP  PPSM  PMSP  PMSM
             22    22    21    21
VACSIG_PRO   PPSP  PPSM  PMSP  PMSM
             16    16    17    17
PHSIGN_NEU         PARTICLES                    HOLES
            1    00    00    00    00        00    00    00    00
PHSIGN_PRO         PARTICLES                    HOLES
            1    00    00    00    00        00    00    00    00
                         ----------  Numerical data  --------
MAX_MULTIP
            2      4      4
COULOMB
            80    79    0.25
SLOW-DOWN
            0.5  0.5
EPS_HERMIT
            1.00E-14
OPTI_GAUSS
            1
GAUSHERMIT
            18    18    32
                         ---  Parameters of the HO basis  ---
BASIS_SIZE
            15    301   800.
HOMEGAZERO
            1.2
SURFAC_PAR
            86    66    1.23
SURFAC_DEF
            2      0    0.61
SURFAC_DEF
            4      0    0.10
                         ----------  Constraints  ----------
OMEGAY
            0.50
MULTCONSTR
            2      0    0.01   42.    1
SPINCONSTR
                   0.00    0.    0
                         ----  Output-file  parameters  ----
PRINT-ITER
            1      0      1
EALLMINMAX
            -12.   0.
                         -------------  Files  -------------
REVIEWFILE
            HFODD.REV
REVIEW
            2
RECORDFILE
            HFODD.REC
REPLAYFILE
            HFODD.REP
WOODSAFILE
            WOODS.WFN
                         -----  Starting the iteration  ----
RESTART
            0
READ_WOODS
            0
NILSSONPAR
            0   -1.175 -0.247   -1.175 -0.352    11.170  11.170  6.280
                         ----------  Calculate  -----------
EXECUTE
                         ----------  Terminate  -----------
ALL_DONE
```

TEST RUN OUTPUT

```
****************************************************************
*                                                              *
*   HFODD    HFODD    HFODD    HFODD    HFODD    HFODD    HFODD    HFODD   *
*                                                              *
****************************************************************
*                                                              *
*          SKYRME-HARTREE-FOCK CODE VERSION 1.60N              *
*         ONE SYMMETRY-PLANE AND NO TIME-REVERSAL SYMMETRY     *
*          DEFORMED CARTESIAN HARMONIC-OSCILLATOR BASIS        *
*                                                              *
****************************************************************
*                                                              *
*             JACEK DOBACZEWSKI AND JERZY DUDEK                *
*         CENTRE DE RECHERCHES NUCLEAIRES, STRASBOURG, 1993-96 *
*                                                              *
****************************************************************
*                                                              *
****************************************************************
*                                                              *
*  CLASSICAL NUCLEAR SURFACE DEFINED FOR:          N = 86   Z = 66 *
*                                                              *
****************************************************************
*                                                              *
*  AL10 =   ZERO  AL11 =   ZERO ............  ............  ............ *
*  AL20 =  0.610  AL21 =   ZERO  AL22 =   ZERO ............  ............ *
*  AL30 =   ZERO  AL31 =   ZERO  AL32 =   ZERO  AL33 =   ZERO ............ *
*  AL40 =  0.100  AL41 =   ZERO  AL42 =   ZERO  AL43 =   ZERO  AL44 =   ZERO *
*                                                              *
****************************************************************
*                                                              *
*                          HOMEGA=  9.2190  FCHOMO=  1.2000    *
*  OSCILLATOR FREQUENCIES: HBAROX= 11.1998  HBAROY= 11.1998  HBAROZ=  6.2464 *
*  MOMENTS OF INERTIA:     XMOMFC= 90.2596  YMOMFC= 90.2596  ZMOMFC= 42.8300 *
*  CENTRES OF MASS:        CMSXFC=  0.0000  CMSYFC=  0.0000  CMSZFC=  0.0000 *
*                                                              *
****************************************************************
*                                                              *
*   PHYSICAL CONSTANTS:      H_BARC=197.32891000    HBCOE2=137.03602000 *
*                           XMASSN=938.90590000    XMASSP=938.27231000 *
*                           HBMASS= 20.73620941    HBMRPA= 20.59978698 *
*                           ECHAR2=  1.43997841    COULEX= -1.06350868 *
*                                                              *
****************************************************************
*                                                              *
*   OSCILLATOR LENGTHS:      X= 1.9243099   Y= 1.9243099   Z= 2.5766958 *
*   OSCILLATOR CONSTANTS:    X= 0.5196668   Y= 0.5196668   Z= 0.3880939 *
*   OSCILLATOR FREQUENCIES:  X=11.1997759   Y=11.1997759   Z= 6.2464470 *
*                                                              *
****************************************************************
*                                                              *
*   BASIS CUT-OFF CONTROL PARAMETERS:  NXMAXX=  8   NYMAXX=  8   NZMAXX=  15 *
*   OPTIMUM NUMBERS OF  GAUSS POINTS:  NXHERM= 18   NYHERM= 18   NZHERM=  32 *
*                                      NLIMIT= 301  LDBASE= 306  MCOUNT=4096 *
*                                      ENECUT= 800.0000    ELIMIT= 112.7539 *
*                                                              *
****************************************************************
*                                                              *
****************************************************************
*                                                              *
*   SHAPE OF THE OSCILLATOR-BASIS DIAMOND                      *
*                                                              *
****************************************************************
*                                                              *
*       NZ ===>>>  0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 *
*       MAX.NX =>  8  8  7  7  6  6  5  4  4  3  3  2  2  1  0  0 *
*                 ---------------------------------------------- *
*   NX= 0  (15)  |  8  8  7  7  6  6  5  4  3  3  2  2  1  0  0   *
*   NX= 1  (13)  |  7  7  6  6  5  5  4  3  3  2  2  1  1  0      *
*   NX= 2  (12)  |  6  6  5  5  4  4  3  2  2  1  1  0  0         *
*   NX= 3  (10)  |  5  5  4  4  3  3  2  1  1  0  0               *
*   NX= 4  ( 8)  |  4  4  3  3  2  2  1  0  0                     *
*   NX= 5  ( 6)  |  3  3  2  2  1  1  0                           *
*   NX= 6  ( 5)  |  2  2  1  1  0  0                              *
*   NX= 7  ( 3)  |  1  1  0  0                                    *
*   NX= 8  ( 1)  |  0  0                                          *
*                                                              *
****************************************************************
*                                                              *
****************************************************************
*                                                              *
* PARAMETER SET SKM*: T0= -2645.00  T1=  410.00  T2=  -135.00  T3= 15595.00 *
* POWER=0.1667 W=130  X0=  0.09000  X1=  0.00000  X2=  0.00000  X3=  0.00000 *
*                                                              *
****************************************************************
```

```
********************************************************************
*                                                                  *
*            COEFFICIENTS DEFINING THE SKYRME FUNCTIONAL            *
*                                                                  *
********************************************************************
*                                                                  *
*              TOTAL(T)       SUM(S)      ISOSCALAR(P)  ISOVECTOR(M) *
*            ----------     --------     ------------  ------------ *
*   CRHO_  =  -1382.012500   780.275000    -991.875000   390.137500 *
*   CRHOD =   1299.583333  -649.791667     974.687500  -324.895833 *
*   CLPR_  =    -85.312500    34.218750     -68.203125    17.109375 *
*   CTAU_  =     68.750000   -68.125000      34.687500   -34.062500 *
*   CSCU_  =      0.000000    68.125000      34.062500    34.062500 *
*   CDIV_  =    -65.000000   -65.000000     -97.500000   -32.500000 *
*                                                                  *
*   CSPI_  =    -59.512500   661.250000     271.112500   330.625000 *
*   CSPID =      0.000000  -649.791667    -324.895833  -324.895833 *
*   CLPS_  =      0.000000    34.218750      17.109375    17.109375 *
*   CCUR_  =    -68.750000    68.125000     -34.687500    34.062500 *
*   CKIS_  =      0.000000   -68.125000     -34.062500   -34.062500 *
*   CROT_  =    -65.000000   -65.000000     -97.500000   -32.500000 *
*                                                                  *
********************************************************************
********************************************************************
*                                                                  *
*  PARITY/SIGNATURE CONFIGURATIONS:                                *
*                                                                  *
*              V A C U U M      P A R T I C L E S       H O L E S   *
*             ===========      =================       ========= *
*             (++) (+-) (-+) (--)  (++) (+-) (-+) (--)  (++) (+-) (-+) (--) *
*                                                                  *
*  NEUTRONS:  22   22   21   21    0    0    0    0    0    0    0    0 *
*  PROTONS :  16   16   17   17    0    0    0    0    0    0    0    0 *
*                                                                  *
********************************************************************
********************************************************************
*                                                                  *
*  CONVERGENCE REPORT                                              *
*                                                                  *
********************************************************************
*                                                                  *
*  ITER    ENERGY    STABILITY     Q20     Q22    SPIN   OMEGA  HOW NICE *
*                                                                  *
*    0   -559.936804 -759.775974   54.178  -0.027  98.777  0.500  0.424287 *
*    1  -1163.385944   88.001030   48.812   0.025  53.243  0.500  1.081832 *
*   48  -1208.769024    0.000468   41.807   0.067  49.581  0.500  1.000000 *
*   49  -1208.768731    0.000400   41.806   0.067  49.581  0.500  1.000000 *
*                                                                  *
********************************************************************
********************************************************************
*                                                                  *
*  SINGLE-PARTICLE PROPERTIES: HARTREE-FOCK            NEUTRONS    *
*                                                                  *
********************************************************************
*                                                                  *
*  NO)    ENERGY (++,+-,-+,--) | N,nz,/\,OMEG>  <P>    JY     SY    GFACT *
*                                                                  *
*  76)  -11.743 ( 0, 0,21, 0) | 5, 3, 2, 3/2>  -100   0.103  -0.092  -0.896 *
*  77)  -11.728 ( 0, 0, 0,20) | 5, 3, 2, 3/2>  -100   0.209  -0.101  -0.485 *
*  78)  -11.433 (19, 0, 0, 0) | 4, 1, 1, 1/2>   100   0.007  -0.182  -3.E+01 *
*  79)  -11.334 ( 0,19, 0, 0) | 4, 1, 3, 5/2>   100  -0.129  -0.040   0.307 *
*  80)  -11.241 (20, 0, 0, 0) | 4, 1, 3, 5/2>   100  -0.100  -0.189   1.885 *
*  81)  -11.137 (21, 0, 0, 0) | 6, 5, 1, 1/2>   100   1.119  -0.176  -0.157 *
*  82)  -11.069 ( 0,20, 0, 0) | 6, 5, 1, 1/2>   100   0.984   0.084   0.086 *
*  83)  -10.881 ( 0,21, 0, 0) | 4, 1, 1, 1/2>   100  -0.112  -0.201   1.784 *
*  84)  -10.379 (22, 0, 0, 0) | 6, 4, 2, 5/2>   100  -0.155  -0.064   0.414 *
*  85)  -10.365 ( 0,22, 0, 0) | 6, 4, 2, 5/2>   100   0.007  -0.024  -3.300 *
*  86)   -9.557 ( 0, 0, 0,21) | 7, 6, 1, 3/2>  -100   2.517   0.041   0.016 *
*  87)   -7.880 ( 0, 0,22, 0) | 5, 2, 1, 3/2>  -100   0.903   0.201   0.222 *
*  88)   -7.840 ( 0, 0, 0,22) | 5, 2, 1, 3/2>  -100   0.442   0.217   0.490 *
*  89)   -7.738 (23, 0, 0, 0) | 4, 0, 2, 5/2>   100  -0.247   0.161  -0.650 *
*  90)   -7.732 ( 0,23, 0, 0) | 4, 0, 2, 5/2>   100  -0.235   0.162  -0.690 *
*  91)   -7.562 ( 0, 0,23, 0) | 5, 2, 1, 3/2>  -100   1.068   0.153   0.144 *
*  92)   -7.221 ( 0, 0, 0,23) | 5, 1, 4, 9/2>  -100  -0.337   0.028  -0.083 *
*  93)   -7.221 ( 0, 0,24, 0) | 5, 1, 4, 9/2>  -100  -0.337   0.028  -0.083 *
*  94)   -7.096 ( 0, 0, 0,24) | 7, 7, 0, 1/2>  -100  -0.134  -0.167   1.252 *
*  95)   -7.076 ( 0,24, 0, 0) | 6, 4, 0, 1/2>   100   1.232   0.328   0.266 *
*  96)   -6.350 ( 0,25, 0, 0) | 4, 0, 0, 1/2>   100   0.078   0.455   5.825 *
*  97)   -6.284 (24, 0, 0, 0) | 6, 3, 3, 7/2>   100   0.140  -0.044  -0.313 *
*                                                                  *
********************************************************************
********************************************************************
*                                                                  *
*            DENSITY INTEGRALS IN THE SKYRME FUNCTIONAL            *
*                                                                  *
********************************************************************
*                                                                  *
*              TOTAL(T)       SUM(S)      ISOSCALAR(P)  ISOVECTOR(M) *
*            ----------     --------     ------------  ------------ *
*   DRHO_  =    17.566618     8.912767      17.566618     0.258917 *
*   DRHOD =    12.488132     6.334617      12.488132     0.181102 *
*   DLPR_  =    -3.719401    -1.886188      -3.719401    -0.052976 *
*   DTAU_  =    15.598603     7.983209      15.598603     0.367815 *
*   DSCU_  =     0.119929     0.064074       0.119929     0.008219 *
*   DDIV_  =     0.823496     0.419204       0.823496     0.014912 *
*                                                                  *
*   DSPI_  =     0.018303     0.010522       0.018303     0.002740 *
*   DSPID =     0.013147     0.007544       0.013147     0.001941 *
*   DLPS_  =    -0.037372    -0.023155      -0.037372    -0.008937 *
*   DCUR_  =     0.060724     0.031580       0.060724     0.002437 *
*   DKIS_  =     0.029460     0.015277       0.029460     0.001094 *
*   DROT_  =     0.007844     0.004322       0.007844     0.000799 *
*                                                                  *
********************************************************************
```

```
****************************************************************
*                                                              *
*          CONTRIBUTIONS TO ENERGY IN THE SKYRME FUNCTIONAL    *
*                                                              *
****************************************************************
*                                                              *
*              TOTAL(T)      SUM(S)      ISOSCALAR(P)  ISOVECTOR(M) *
*              --------      ------      ------------  ------------ *
*   ERHO_  =  -24277.285107   6954.409417  -17423.888833    101.013143 *
*   ERHOD =   16229.367796  -4116.181326   12172.025847    -58.839377 *
*   ELPR_  =     317.311377    -64.543010     253.674755     -0.906388 *
*   ETAU_  =    1072.403924   -543.856103     541.076525    -12.528704 *
*   ESCU_  =       0.000000      4.365047       4.085077      0.279970 *
*   EDIV_  =     -53.527218    -27.248236     -80.290827     -0.484627 *
*              ============  ============  ============  ============ *
*   SUM EVEN:  -6711.729227   2206.945789   -4533.317455     28.534017 *
*                                                              *
*   ESPI_  =      -1.089276      6.957479       4.962258      0.905945 *
*   ESPID =        0.000000     -4.901833      -4.271249     -0.630584 *
*   ELPS_  =       0.000000     -0.792320      -0.639413     -0.152907 *
*   ECUR_  =      -4.174748      2.151393      -2.106350      0.082995 *
*   EKIS_  =       0.000000     -1.040747      -1.003485     -0.037261 *
*   EROT_  =      -0.509892     -0.280907      -0.764838     -0.025961 *
*              ============  ============  ============  ============ *
*   SUM  ODD:     -5.773917      2.093065      -3.823078      0.142226 *
*                                                              *
****************************************************************
****************************************************************
*                                                              *
*  MULTIPOLE MOMENTS IN UNITS OF (10 FERMI)**LAMBDA       TOTAL *
*                                                              *
****************************************************************
*                                                              *
*  Q00 =152.0000  ............  ............  ............  ............ *
*                                                              *
*  Q10 =    ZERO  Q11 =    ZERO  ............  ............  ............ *
*                                                              *
*  Q20 = 41.8059  Q21 =    ZERO  Q22 =  0.0675  ............  ............ *
*                                                              *
*  Q30 =    ZERO  Q31 =    ZERO  Q32 =    ZERO  Q33 =    ZERO  ............ *
*                                                              *
*  Q40 =  4.7902  Q41 =    ZERO  Q42 =  0.0058  Q43 =    ZERO  Q44 = -0.0011 *
*                                                              *
****************************************************************
*                                                              *
*  ROOT-MEAN-SQUARE AND GEOMETRIC SIZES IN FERMIS         TOTAL *
*                                                              *
*  R_RMS =  5.5420   X_RMS =  2.3844   Y_RMS =  2.3712   Z_RMS =  4.4052 *
*                                                              *
*  R_GEO =  7.1547   X_GEO =  5.3318   Y_GEO =  5.3022   Z_GEO =  9.8504 *
*                                                              *
****************************************************************
*                                                              *
*  ANGULAR MOMENTA AND THE FIRST MOMENTS OF INERTIA FOR OMEGA = 0.500000 MEV *
*                                                              *
****************************************************************
*                                                              *
*                      SPINS                     J(1)          *
*             ------------------------   ------------------------ *
*              ORBITAL  INTRINSIC  TOTAL   ORBITAL  INTRINSIC  TOTAL *
*   NEUTRONS   28.21798   1.21125  29.42923   56.43596   2.42250  58.85846 *
*   PROTONS    19.29890   0.85368  20.15257   38.59779   1.70736  40.30515 *
*   --------                                                    *
*   TOTAL      47.51687   2.06493  49.58181   95.03375   4.12986  99.16361 *
*                                                              *
****************************************************************
*                                                              *
*                   NEUTRON  CONFIGURATIONS                    *
*                   =======================                    *
*       P S  12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 *
*       ---  ---------------------------------------------------------------- *
*   CONF: + +   1  1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0 *
*   VACC: + +   1  1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0 *
*   CONF: + -   1  1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0 *
*   VACC: + -   1  1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0 *
*   CONF: - +   1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0  0 *
*   VACC: - +   1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0  0 *
*   CONF: - -   1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0  0 *
*   VACC: - -   1  1  1  1  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0  0 *
*                                                              *
****************************************************************
*                                                              *
*                       ENERGIES (MEV)                        *
*                                                              *
****************************************************************
*                                                              *
*  KINETIC: (NEU)=  1652.730622   (PRO)=  1107.885480   (TOT)=  2760.616103 *
*  SUM EPS: (NEU)= -2034.973323   (PRO)= -1133.181733   (TOT)= -3168.155056 *
*  PAIRING: (NEU)=     0.000000   (PRO)=     0.000000   (TOT)=     0.000000 *
*                                                              *
*  COULOMB: (DIR)=   564.434280   (EXC)=   -25.354572   (TOT)=   539.079708 *
*                                                              *
*  CONSTR. (MULT)=     0.000377   SLOPE=    -0.003881   CORR.=    -0.081133 *
*  CONSTR. (SPIN)=   -24.790903   SLOPE=     0.500000   CORR.=   -12.395451 *
*                                                              *
*  REARRANGEMENT ENERGY FROM THE SKYRME DENSITY-DEPENDENT TERMS=  1009.023720 *
*  ROUTHIAN  (TOTAL ENERGY PLUS MULTIPOLE AND SPIN CONSTRAINTS)= -1233.559005 *
*                                                              *
*  SPIN-ORB (EVE)=   -80.775454   (ODD)=    -0.790799   (TOT)=   -81.566253 *
*  SKYRME:  (EVE)= -4504.783438   (ODD)=    -3.680852   (TOT)= -4508.464290 *
*                                                              *
*  TOTAL:   (STAB)=     0.000343   (SP)= -1208.768136   (FUN)= -1208.768479 *
*                                                              *
****************************************************************
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Table 1: Precision of results obtained for various observables calculated by the code HFODD with the physical basis parameters and $M=300$. Absolute values correspond to the results for ^{152}Dy and ^{208}Pb, while the relative values correspond to the differences between ^{151}Tb and ^{152}Dy. The values denoted as "precision" represent also typical orders of magnitude of the accuracy obtained in other cases for the same numerical conditions.

	Absolute values		Relative values	
Observable	Precision	%	Precision	%
Energy $\mathcal{E}$	5 MeV	0.4%	0.05 MeV	1%
Radius R_{rms}	0.003 fm	0.05%	—	—
Quadrupole moment Q_p	0.05 b	0.3%	0.01 b	1%
Angular momentum I	0.1 $\hbar$	0.2%	0.03 $\hbar$	2%
Static moment $\mathcal{J}^{(1)}$	0.2 $\hbar^2$/MeV	0.2%	0.06 $\hbar^2$/MeV	2%
Dynamic moment $\mathcal{J}^{(2)}$	0.1 $\hbar^2$/MeV	0.1%	0.1 $\hbar^2$/MeV	2-10%

Figure 1: Ground-state energies of ^{208}Pb (solid lines) calculated as functions of $\hbar\omega_0$ for several values of the number N_0 of HO shells included in the basis. Dots denote the minima, the asterisk gives the value calculated at N_0=20 for the physical value of $\hbar\omega_0$ shown by the vertical dashed line. The horizontal dashed line represents the exact result.

Figure 2: Same as in Fig. 1 but for the rms radii of ^{208}Pb.

Figure 3: Energies of superdeformed state in ^{152}Dy (solid lines) calculated at $\hbar\omega$=0 as functions of the basis deformation parameter q for several values of the number M of states included in the HO basis. Dots denote the minima, the asterisk gives the value calculated at M=1200 for the physical value of q shown by the vertical dashed line. The horizontal dashed line represents the exact result, see text.

Figure 4: Same as in Fig. 3 but for the proton quadrupole moments Q_p of superdeformed ^{152}Dy at $\hbar\omega$=0.

Figure 5: Angular momenta of the rotating superdeformed nucleus ^{152}Dy (solid lines) calculated at $\hbar\omega$=0.5 MeV as functions of the basis deformation parameter q for several values of the number M of states included in the HO basis. Dots denote the minima of the Routhian (I-21), the asterisk and the horizontal dashed line gives the value calculated at M=1200 for the physical value of q shown by the vertical dashed line.

Figure 6: Same as in Fig. 5 but for the dynamic moment $\mathcal{J}^{(2)}$ (7) of superdeformed ^{152}Dy at $\hbar\omega$=0.55 MeV.

Figure 7: Proton separation energies in SD ^{152}Dy (solid lines) relative to the SD state in ^{151}Tb, i.e., the differences of energies $\mathcal{E}^{\text{SD}}(^{151}\text{Tb})-\mathcal{E}^{\text{SD}}(^{152}\text{Dy})$, obtained at $\hbar\omega$=0. Solid lines denote values calculated as functions of the basis deformation parameter q for several values of the number M of states included in the HO basis. Dots denote the minima of the energy in ^{152}Dy (Fig. 3), the asterisk and the horizontal dashed line gives the value calculated at M=1200 for the physical value of q shown by the vertical dashed line.

Figure 8: Same as in Fig. 7 but for the quadrupole polarizations induced in the ^{152}Dy core by the $\pi[651](3/2)(+i)$ hole, i.e., the differences of proton quadrupole moments $Q_p^{\text{SD}}(^{151}\text{Tb})-Q_p^{\text{SD}}(^{152}\text{Dy})$.

Figure 9: Same as in Fig. 7 but for the relative alignments between the ^{151}Tb and ^{152}Dy nuclei, i.e., the differences of angular momenta $I(^{151}\text{Tb})-I(^{152}\text{Dy})$ at $\hbar\omega$=0.5 MeV.
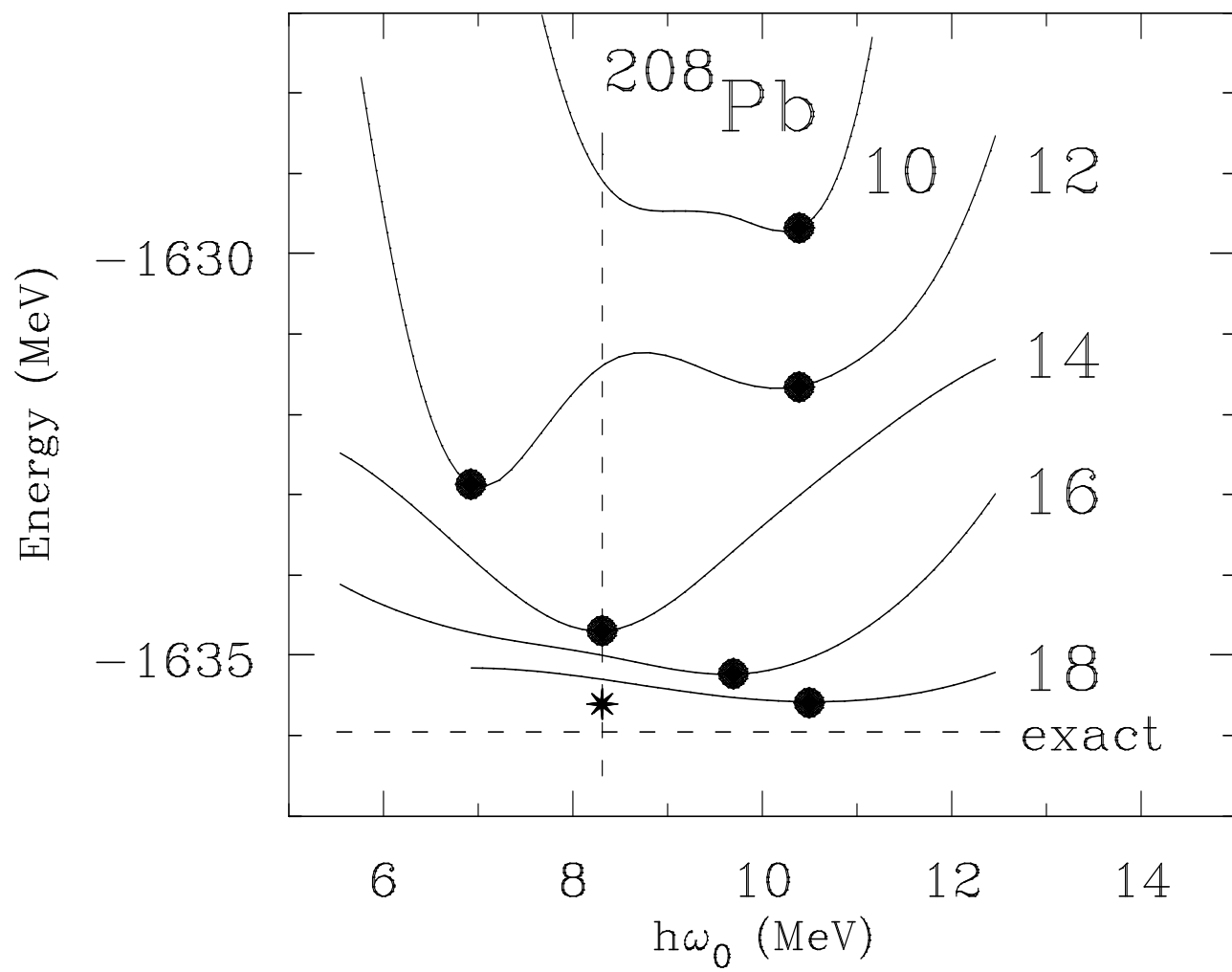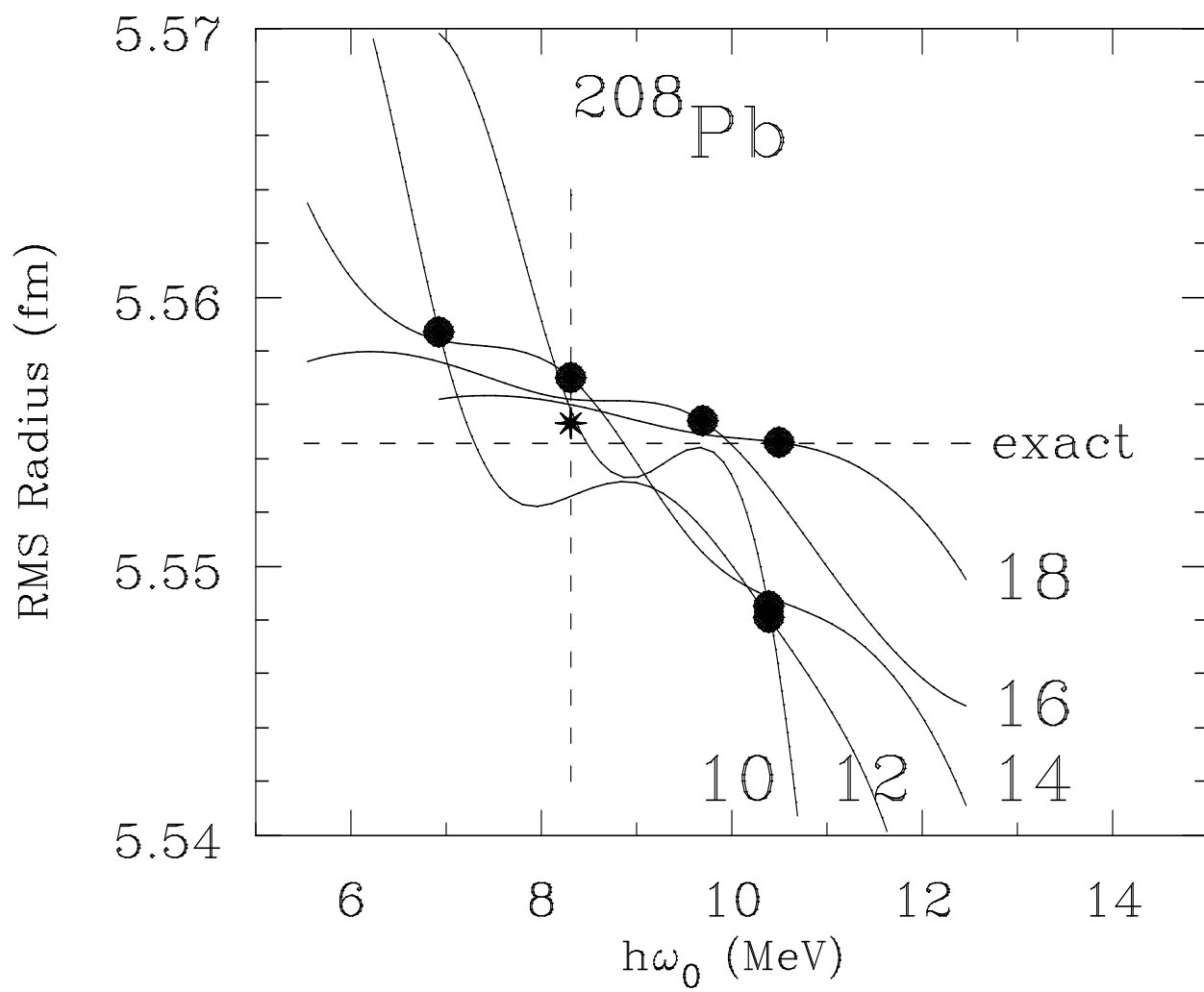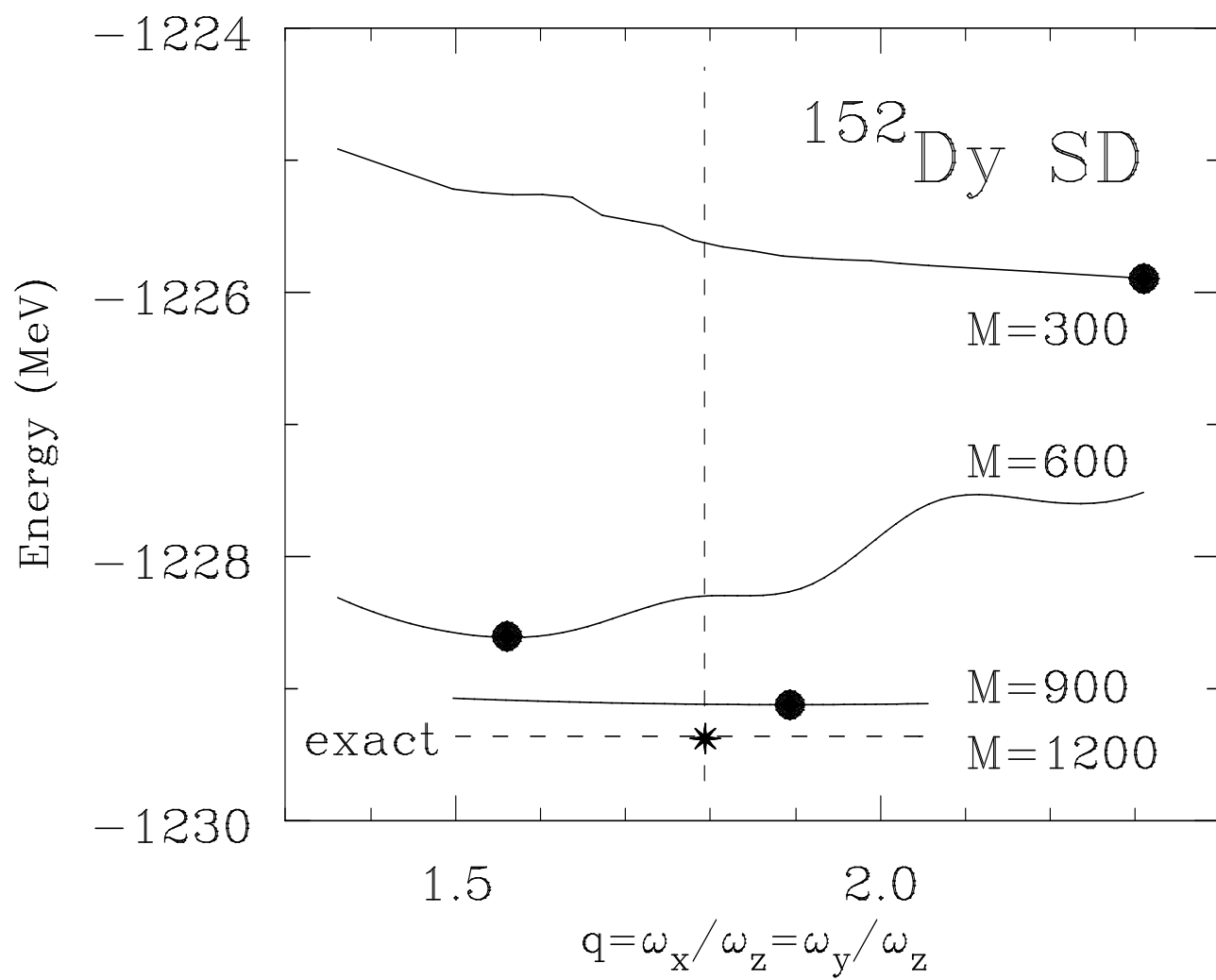
Figure 1.

Figure 2.

Figure 3.

Figure 4.
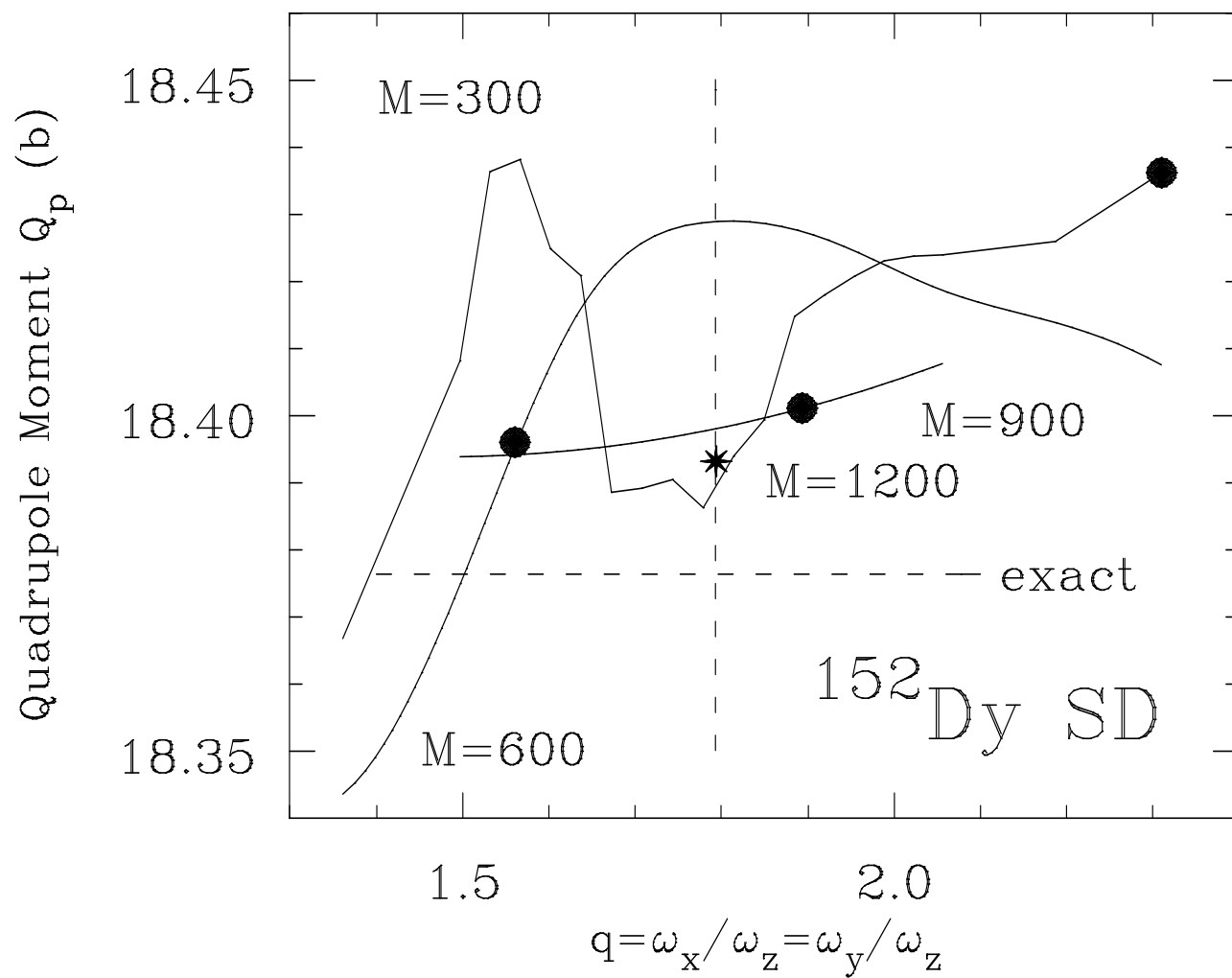
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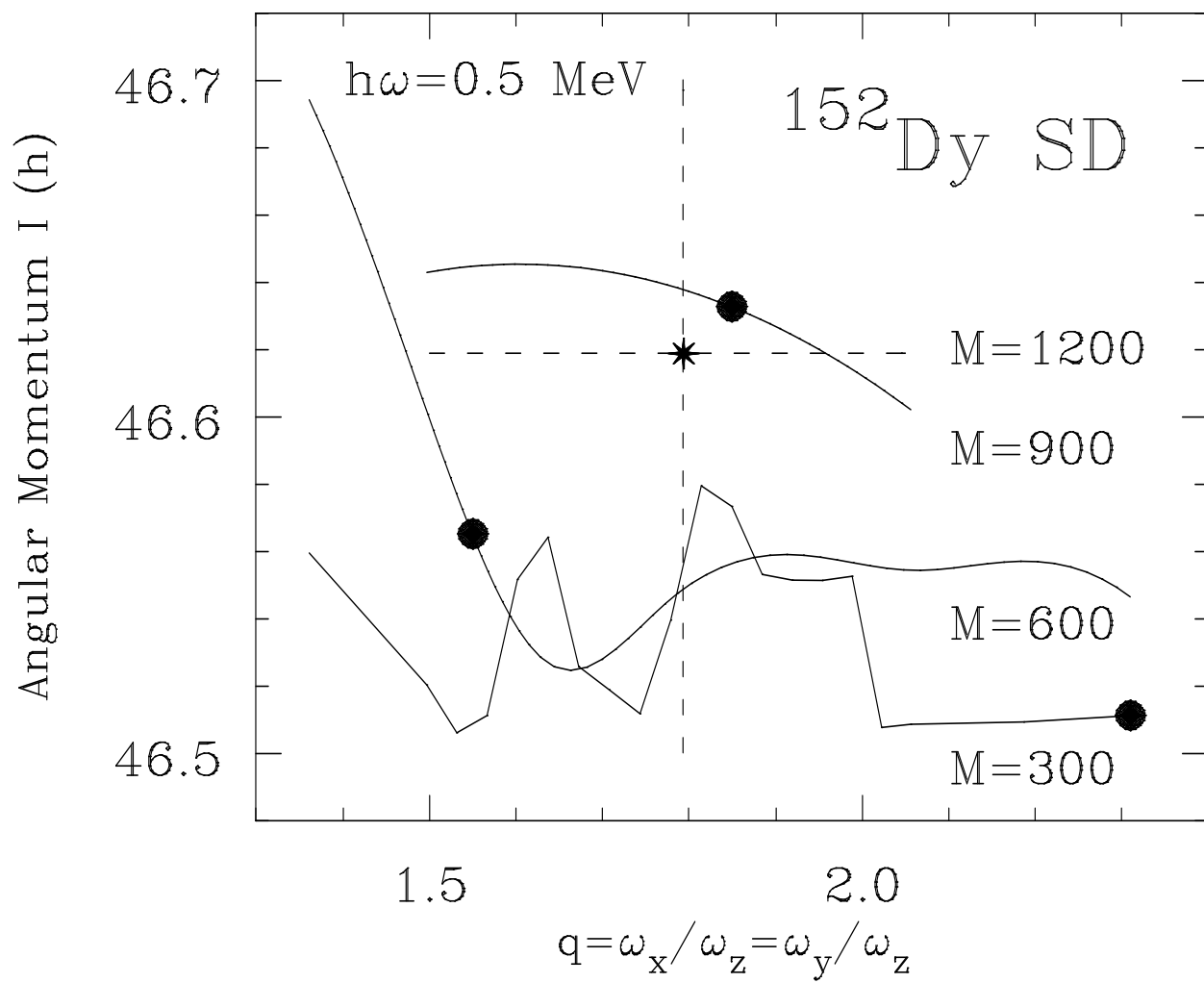
Figure 6.
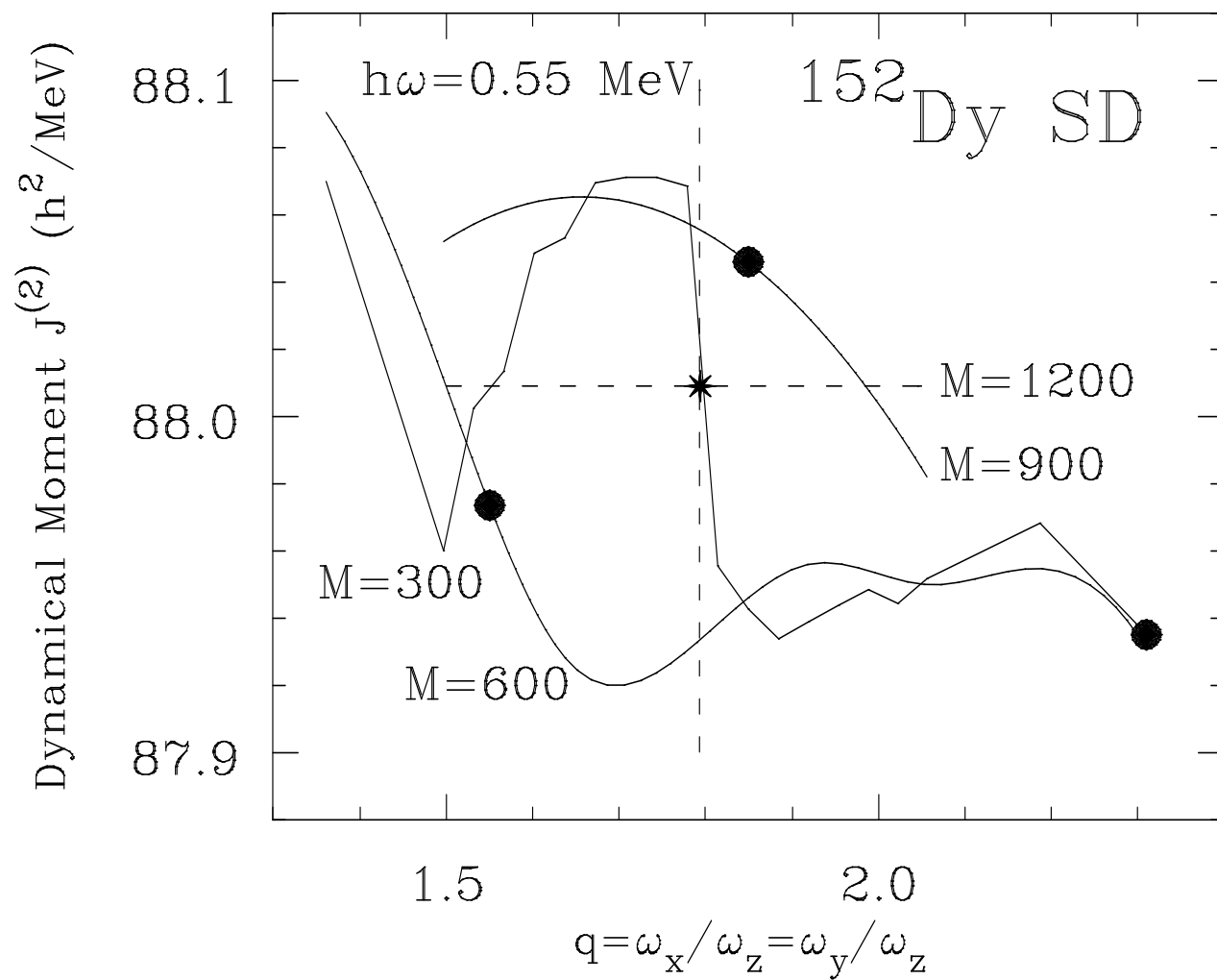
Figure 7.

Figure 8.

Figure 9.